Self-adjoint differential operators assosiated with self-adjoint differential expressions

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Abstract

Considerable attention has been recently focused on quantum-mechanical systems with boundaries and/or singular potentials for which the construction of physical observables as self-adjoint (s.a.) operators is a nontrivial problem. We present a comparative review of various methods of specifying ordinary s.a. differential operators generated by formally s.a. differential expressions based on the general theory of s.a. extensions of symmetric operators. The exposition is untraditional and is based on the concept of asymmetry forms generated by adjoint operators. The main attention is given to a specification of s.a. extensions by s.a. boundary conditions. All the methods are illustrated by examples of quantum-mechanical observables like momentum and Hamiltonian. In addition to the conventional methods, we propose a possible alternative way of specifying s.a. differential operators by explicit s.a. boundary conditions that generally have an asymptotic form for singular boundaries. A comparative advantage of the method is that it allows avoiding an evaluation of deficient subspaces and deficiency indices. The effectiveness of the method is illustrated by a number of examples of quantum-mechanical observables.

1 Introduction

Among the problems of quantum description of physical systems and its proper interpretation, there is the problem of a correct definition of observables as self-adjoint (s.a. in what follows) operators in an appropriate Hilbert space. This problem is highly nontrivial for physical systems with boundaries and/or with singular interactions (including QFT models); for brevity, we call such systems nontrivial physical systems. The interest in this problem is periodically revived in connection with one or another particular physical system. The reason is that the solution of this problem and consequently a consistent quantum-mechanical treatment of nontrivial systems requires appealing to some nontrivial chapters of functional analysis concerning the theory of unbounded linear operators, but the content of such chapters is usually beyond the scope of the mathematical apparatus given in standard text-books on quantum mechanics for physicists[1]. A crucial subtlety is that an unbounded operator, in particular, a quantum-mechanical observable, cannot be defined in the whole Hilbert space, i.e., for any quantum-mechanical state. But "there is no operator without its domain of definition", an operator is not only a "rule of

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[1] The exceptions like [1, 2, 3] are mainly intended for mathematicians.

acting", but also a domain in a Hilbert space, to which this rule is applicable. In the case of unbounded operators, the same rule for different domains defines different operators with sometimes crucially different properties. It is a proper choice of the domain for a quantum-mechanical observable that makes it a s.a. operator. The main problems are related exactly with this task.

The formal rules of canonical quantization are of preliminary nature and generally provide only, so to speak, "candidates" for unbounded quantum-mechanical observables, for example, formally s.a. differential expressions[2], because their domains are not prescribed by the quantization rules and are not even clear at the first stage of quantization, especially for nontrivial physical systems, even though it is prescribed that observables must be s.a. operators.

We would like to elucidate our understanding of this point. The choice of domains providing the self-adjointness of all observables involved, especially of primarily important observables like position, momentum, Hamiltonian, symmetry generators, is a necessary part of quantization resulting in a specification of quantum-mechanical description of a physical system under consideration; this is actually a physical problem. Mathematics can only help a physicist in this choice indicating various possibilities.

It appears that for physical systems whose classical description incorporates infinite plane phase spaces like $\mathbb{R}^{2n}$ and "regular" interactions, quantization is practically unique: the most important physical observables are defined as s.a. operators on some "natural" domains, in particular, classical symmetries can be conserved in a quantum description. The majority of textbooks begin their exposition of quantum mechanics exactly with the treatment of such physical systems. Of course, nontrivial physical systems are also considered afterwards. But the common belief is that no actual singularities exist in Nature. They are the products of our idealization of reality, i.e., are of a model nature, for example, related to our ignorance of the details of an interaction at small distances. We formally extend an interaction law known for finite distances between finite objects to infinitely small distances between point-like objects. We treat boundaries as a result of infinite potential walls that are actually always finite[3]. The consequence is that singular problems in quantum mechanics are commonly solved via some regularization that is considered natural and then by a following limiting process of removing the regularization. However, in some cases the so-called infinite renormalization (of "charges", for example) is required. Moreover, in some cases there exists no reasonable limit. (We should emphasize that we speak here about conventional quantum mechanics, rather than about quantum field theory.) It can also happen that physical results are unstable under regularization: different regularizations yield different physical results. It is exactly in these cases that mathematics can help a physicist with the theory of s.a. extensions of symmetric operators. This was first recognized by Berezin and Faddeev [4] in connection with the three-dimensional δ-potential problem.

The practice of the quantization of nontrivial systems shows that preliminary candidates for observables can be quite easily assigned symmetric operators defined on the domains that "avoid" the problems: they do not "touch" boundaries and "escape" singularities of interaction; this is a peculiar kind of "mathematical regularization". However such symmetric operators are commonly non-self-adjoint. The main question then is whether these preliminary observables can be assigned s.a. operators by extensions which make the candidates real observables. The answer is simple if a symmetric operator under consideration is bounded. But if it is unbounded,

[2]S.a. according to Lagrange in mathematical terminology, see below sec.2.

[3]To be true, a plane infinite space is also an idealization, as any infinity.

the problem is generally nontrivial.

The theory of s.a. extensions of unbounded symmetric operators is the main tool in solving this problem. It appears that in general these extensions are highly nonunique if at all possible. For physics, this implies that there are many quantum mechanical descriptions of the same nontrivial physical system. The general theory shows all the possibilities that mathematics can present to a physicist for his choice. Of course, the physical interpretation of available s.a. extensions is a purely physical problem. Any extension is a certain prescription for the behavior of a physical system under consideration near boundaries and singularities. We also believe that each extension can be understood through an appropriate regularization and limiting process, although this in itself is generally a complicated problem. But, in any case, the right of a final choice belongs to a physicist.

The general theory of extensions of unbounded symmetric operators is mainly due to von Neumann [5] (An English exposition of von Neumann's paper can be found in [6]). We expound only a necessary part of this theory that concerns the case of s.a. extensions.

The following three theorems exhaust the content of the necessary part of the theory. They bear no name in the conventional mathematical literature [7, 8]; instead, their crucial formulas are called the von Neumann formulas. We call these theorems the respective first and second von Neumann theorems and the main theorem[4].

We attempt to make our exposition maximally self-contained as far as possible and first remind a reader the basic notions and facts, but only those that are absolutely necessary for understanding the main statements; there are many books on the subject. We mainly refer to [7, 8] although follow an alternative way of describing s.a. extensions of symmetric operators. The final statements are our guides in constructing quantum-mechanical observables.

The article is organized as follows: In Sec. 2, we remind of the general theory of symmetric extensions of unbounded symmetric operators. The exposition is untraditional and is based on the notion of asymmetry forms generated by adjoint operators. The basic statements concerning the possibility and specification of s.a. extensions both in terms of isometries between the deficient subspaces and in terms of the sesquilinear asymmetry form are collected in the main theorem. (There follows a comment on a direct application of the main theorem to physical problems of quantization.) We outline a possible general scheme of constructing quantum-mechanical observables as s.a. operators starting from initial formal expressions supplied by canonical quantization rules. The scheme is illustrated by the example of the momentum operator for a particle moving on different intervals of the real axis (the whole real axis, a semiaxis, a finite interval). Sec. 3 is devoted to the exposition of specific features and appropriate modifications of the general theory as applied to ordinary s.a. differential operators in Hilbert spaces $L^2(a, b)$ associated with formal differential expressions s.a. according to Lagrange. For differential operators, the isometries between deficient subspaces specifying s.a. extensions can be converted to s.a. boundary conditions, explicit or implicit, based on the fact that asymmetry forms are expressed in terms of the (asymptotic) boundary values of functions and their derivatives. We describe various ways of specifying s.a. operators associated with s.a. differential expressions by s.a. boundary conditions depending on the regularity or singularity of the boundaries of the interval under consideration. All the methods are illustrated by examples of quantum-mechanical observables like momentum and Hamiltonian. In addition to the known conventional methods, we discuss a possible alternative way of specifying s.a. differential oper-

[4] A reader interested in the final statement (without the details of a strict proof) can go directly to the main theorem, Theorem 3, and the subsequent comments placed at the end of Sec. 2.

ators by explicit s.a. boundary conditions that generally have an asymptotic form for singular boundaries. A comparative advantage of the method is that it allows avoiding the evaluation of deficient subspaces and deficiency indices. Its effectiveness is illustrated by a number of examples of quantum-mechanical observables.

2 Basics of theory of symmetric operators

2.1 Generalities

We begin with a notation.

Let $\mathcal{H}$ be a Hilbert space, its vectors are denoted by Greek letters: $\xi, \eta, ..., \psi \in \mathcal{H}$. The symbol (η, ξ) denotes a scalar product in $\mathcal{H}$; by the physical tradition, the scalar product is linear in the second argument and anti-linear in the first one.

Let M be a subspace in $\mathcal{H}$, $M \subset \mathcal{H}$, then its closure and its orthogonal complement are respectively denoted by $\overline{M}$ and $M^{\perp}$, M is a closed subspace if $M = \overline{M}$. For any M, the decomposition $\mathcal{H} = \overline{M} \oplus M^{\perp}$ holds, where $\oplus$ is the symbol of a direct orthogonal sum, i.e., any vector $\xi \in \mathcal{H}$ is uniquely represented as

$$\xi = \underline{\xi} + \xi^{\perp}\,, \ \underline{\xi} \in \overline{M}\,, \ \xi^{\perp} \in M^{\perp}\,.$$

A subspace M is called dense in $\mathcal{H}$ if $\overline{M} = \mathcal{H}$, then $M^{\perp} = \{0\}$.

Operators in $\mathcal{H}$, we consider only linear operators, are denoted by the Latin letters $\hat{f}$, $\hat{g}$, ... with a hat above. Their domains and ranges are subspaces in $\mathcal{H}$ and are respectively denoted by D_f, D_g, ... and R_f, R_g, ... The unit, or identity, operator is denoted by $\hat{I}$. An operator $\hat{f}$ is called densely defined[5] if $\overline{D_f} = \mathcal{H}$.

An operator $\hat{f}$ is defined by its graph

$$\mathbb{G}_f = \left\{ \begin{pmatrix} \xi \\ \eta = \hat{f}\,\xi \end{pmatrix} \right\} \subset \mathbb{H} = \mathcal{H} \oplus \mathcal{H}\,, \ \forall \xi \in D_f\,, \ \eta \in R_f\,,$$

a subspace in the direct orthogonal sum of two copies of $\mathcal{H}$, ξ is an abscissa of the graph, η is its ordinate. The scalar product of two vectors $\mathbf{v}_1 = \begin{pmatrix} \xi_1 \\ \eta_1 \end{pmatrix} \in \mathbb{H}$ and $\mathbf{v}_2 = \begin{pmatrix} \xi_2 \\ \eta_2 \end{pmatrix} \in \mathbb{H}$ is defined by $(\mathbf{v}_1, \mathbf{v}_2) = (\xi_1, \xi_2) + (\eta_1, \eta_2)$. Two operators $\hat{f}$ and $\hat{g}$ are equal if $\mathbb{G}_f = \mathbb{G}_g$, in particular, $D_f = D_g$.

We assume that the notion of sum $\hat{f} + \hat{g}$ of operators, $D_{f+g} = D_f \cap D_g$, and the notion of the multiplication of an operator by a complex number z, i.e., $\hat{f} \to z\hat{f}$, $D_{zf} = D_f$, are known; in particular, $D_{f-zI} = D_f$.

The kernel of an operator $\hat{f}$ is defined as the subspace of null-vectors of the operator, $\ker \hat{f} = \left\{ \xi \in D_f : \hat{f}\,\xi = 0 \right\}$. If $\ker \hat{f} = \{0\}$, the operator $\hat{f}$ is invertible, i.e., there exists the inverse operator, or simply inverse, $\hat{f}^{-1}$ whose graph $\mathbb{G}_{f^{-1}}$ is

$$\mathbb{G}_{f^{-1}} = \left\{ \begin{pmatrix} \eta = \hat{f}\,\xi \\ \hat{f}^{-1}\eta = \xi \end{pmatrix} \right\},$$

[5] Actually, only such operators are interesting for quantum mechanics.

where abscissas and ordinates are interchanged with respect to $\mathbb{G}_f$ such that $D_{f^{-1}} = R_f$ and $R_{f^{-1}} = D_f$. It is evident that $\left(\hat{f}^{-1}\right)^{-1} = \hat{f}$.

We assume that the notions of the operator norm, of bounded, or continuous, and unbounded operators are known.

An operator $\hat{g}$ is called an extension of an operator $\hat{f}$ if $\mathbb{G}_f \subset \mathbb{G}_g$, i.e., if $D_f \subset D_g$ and $\hat{g}\xi = \hat{f}\xi$, $\forall \xi \in D_f$, the operator $\hat{f}$ is respectively called the restriction of $\hat{g}$; this is written as $\hat{f} \subset \hat{g}$. A bounded continuous operator can be extended to the whole $\mathcal{H}$ with the same norm.

For an unbounded operator, the notion of continuity is replaced by the notion of closedness; for many purposes, it is sufficient that an operator be closed. An operator $\hat{f}$ is called closed, which is written as $\hat{f} = \overline{\hat{f}}$, if its graph is closed, $\mathbb{G}_f = \overline{\mathbb{G}_f}$, as a subspace in $\mathbb{H}$, i.e., $\xi_n \to \xi,\ \hat{f}\xi_n \to \eta,\ \{\xi_n\}_1^\infty \subset D_f \Longrightarrow \xi = D_f,\ \eta = \hat{f}\xi$. The difference between closedness and continuity is that not any convergent sequence $\{\xi_n\}_1^\infty \subset D_f$ yields a convergent sequence $\left\{\hat{f}\xi_n\right\}_1^\infty$, the latter can diverge, but it is not allowed for two sequences $\left\{\hat{f}\xi_n^{(1)}\right\}_1^\infty$ and $\left\{\hat{f}\xi_n^{(2)}\right\}_1^\infty$ to converge to different limits if the sequences $\left\{\xi_n^{(1)}\right\}_1^\infty$ and $\left\{\xi_n^{(2)}\right\}_1^\infty$ have the same limit. If an operator $\hat{f}$ is bounded and closed, its domain is a closed subspace, $D_f = \overline{D_f}$; if $\hat{f}$ is closed and invertible, its inverse is also closed, $\hat{f}^{-1} = \overline{\hat{f}^{-1}}$; for a closed operator, we also have $\overline{\hat{f} - z\hat{I}} = \hat{f} - z\hat{I}$. It is remarkable that a closed It is remarkable that a closed operator defined everywhere is bounded (the theorem on a closed graph), therefore, a closed unbounded operator defined everywhere is impossible. An operator $\hat{f}$ by itself can be nonclosed, but allow the closure, or be closable. A generally nonclosed operator $\hat{f}$ is called closable if it allows a closed extension; the minimum closed extension is called the closure[6] of $\hat{f}$ and is denoted by $\overline{\hat{f}}$, $\hat{f} \subseteq \overline{\hat{f}}$, its graph $\mathbb{G}_{\bar{f}} = \overline{\mathbb{G}_{\hat{f}}}$, the closure of $\mathbb{G}_f$ in $\mathbb{H}$. Of course, any graph can be made closed, $\mathbb{G}_f \to \overline{\mathbb{G}_f}$ but the closure $\overline{\mathbb{G}_f}$ must remain a graph, i.e., a subspace in $\mathbb{H}$ where any abscissa uniquely determines an ordinate, which is nontrivial.

Any densely defined (and only densely defined) operator $\hat{f}$ is assigned the adjoint operator, or simply adjoint, $\hat{f}^+$. Its graph[7] $\mathbb{G}_{f^+}$ is $\mathbb{G}_{f^+} = (i\sigma^2\mathbb{G}_f)^\perp$ (the orthogonal complement is taken in $\mathbb{H}$); equivalently, $\hat{f}^+$ is defined by the equation

$$\left(\xi_*, \hat{f}\xi\right) - \left(\eta_* = \hat{f}^+\xi_*, \xi\right) ,\ \forall \xi \in D_f ,$$

for the pairs of vectors $\xi_* \in D_{f^+}$ and $\eta_* = \hat{f}^+\xi_* \in R_{f^+}$ constituting the graph of $\hat{f}^+$. We call this equation the defining equation for $\hat{f}^+$ and only note that $\hat{f}^+$ must be evaluated. It is evident that[8] $\left(z\hat{f}\right)^+ = \overline{z}\hat{f}^+$. The adjoint $\hat{f}^+$ is always closed because any orthogonal complement is a closed subspace. It is important that an extension of a densely defined operator is accompanied by a restriction of its adjoint: $\hat{f} \subset \hat{g} \Longrightarrow \hat{g}^+ \subseteq \hat{f}^+$. The closure of a densely defined operator, if it exists, has the same adjoint, $\left(\overline{\hat{f}}\right)^+ = \hat{f}^+$. A densely defined operator $\hat{f}$ is closable iff[9] its

[6] The fundamental notions of a closed operator and closability are usually left aside in physical textbooks, probably because even though not any operator allows a closure, such "pathologic" operators are not encountered in physics.

[7] Here and elsewhere σ^k, $k = 1, 2, 3$ denote Pauli matrices.

[8] The bar over numerical quantities denotes complex conjugation.

[9] Iff means "if and only if".

adjoint is also densely defined, $\overline{D_{f^+}} = \mathcal{H}$, and if so, the equality $\overline{\hat{f}} = \left(\hat{f}^+\right)^+$ holds. We note that the generally accepted equality $\left(\hat{f}^+\right)^+ = \hat{f}$ holds only for closed operators. We also note that generally $\left(\hat{f} + \hat{g}\right)^+ \neq \hat{f}^+ + \hat{g}^+$ for densely defined unbounded operators: $\left(\hat{f} + \hat{g}\right)^+$ may not exist if $\overline{D_f \cap D_g} \neq \mathcal{H}$, and even if $\overline{D_f \cap D_g} = \mathcal{H}$, we generally have $\hat{f}^+ + \hat{g}^+ \subseteq \left(\hat{f} + \hat{g}\right)^+$. But if one of the operators, let it be $\hat{g}$, is bounded and defined everywhere, the generally accepted equality $\left(\hat{f} + \hat{g}\right)^+ = \hat{f}^+ + \hat{g}^+$ holds, in particular, $\left(\hat{f} - z\hat{I}\right)^+ = \hat{f}^+ - \overline{z}I$. For a densely defined operator $\hat{f}$, the equality $R_f^\perp = \ker \hat{f}^+$ holds, which implies the decomposition $\mathcal{H} = \overline{R_f} \oplus \ker \hat{f}^+$, in particular, $\mathcal{H} = \overline{R_{f-zI}} \oplus \ker\left(\hat{f}^+ - \overline{z}I\right)$. If $\hat{f}$ and $\hat{f}^+$ are invertible, the equality $\left(\hat{f}^{-1}\right)^+ = \left(\hat{f}^+\right)^{-1}$ holds.

2.2 Self-adjoint and symmetric operators, deficiency indices

A densely defined operator $\hat{f}$ is called s.a. if it coincides with its adjoint $\hat{f}^+$, $\hat{f} = \hat{f}^+$, i.e., $\mathbb{G}_f = \mathbb{G}_{f^+}$, in particular, $D_f = D_{f^+}$. All quantum-mechanical observables are s.a. operators. A s.a. operator is evidently closed. Therefore, any bounded s.a. operator is defined everywhere, but an unbounded s.a. operator cannot be defined everywhere. This concerns the majority of quantum-mechanical observables and generates one of the main problems of quantization. One of the obstacles is that the sum of two unbounded s.a. operators $\hat{f} = \hat{f}^+$, and $\hat{g} = \hat{g}^+$ is generally non-s.a.: even if $\overline{D_f \cap D_g} = \mathcal{H}$, we generally have $\hat{f} + \hat{g} \subseteq \left(\hat{f} + \hat{g}\right)^+$. But if one of the operators, let it be $\hat{g}$, is a bounded s.a. operator, the sum $\hat{f} + \hat{g}$ is a s.a. operator with the domain $D_{f+g} = D_f$, in particular, $\hat{f} - \lambda\hat{I} = \left(\hat{f} - \lambda\hat{I}\right)^+$ for $\lambda = \overline{\lambda}$. It follows from the previous remarks that a s.a. operator $\hat{f}$ does not allow s.a. extensions, and if it is invertible, its inverse $\hat{f}^{-1}$ is also a s.a. operator.

The requirement of self-adjointness is a rather strong requirement.

A less restrictive notion is the notion of symmetric operator[10]. An operator $\hat{f}$ is called symmetric if $\hat{f}$ is densely defined, $\overline{D_f} = \mathcal{H}$, and if the equality

$$\left(\eta, \hat{f}\xi\right) = \left(\hat{f}\eta, \xi\right), \ \forall \xi, \eta \in D_f \tag{1}$$

holds. An equivalent definition of a symmetric operator $\hat{f}$ is that it is densely defined and its adjoint $\hat{f}^+$ is an extension of $\hat{f}$, $\hat{f} \subseteq \hat{f}^+$, i.e., $\mathbb{G}_f \subseteq \mathbb{G}_{f^+}$, in particular, $D_f \subseteq D_{f^+}$. A s.a. operator is a symmetric operator with an additional property $D_f = D_{f^+}$. The problem, we are interested in all what follows is whether a given symmetric operator allows s.a. extensions.

We list the basic properties of symmetric operators that are used below. They directly follow from the aforesaid or can be found in [7, 8].

Any symmetric operator $\hat{f}$ has a symmetric closure $\overline{\hat{f}}$ such that the chain of inclusions $\hat{f} \subseteq \overline{\hat{f}} = \left(\hat{f}^+\right)^+ \subseteq \left(\overline{\hat{f}}\right)^+ = \hat{f}^+$ holds, in particular, $\hat{f}^+\underline{\xi} = \overline{\hat{f}}\underline{\xi}$ for any vector $\underline{\xi} \in D_{\overline{f}}$.

Therefore, when setting the problem of symmetric extensions, especially, s.a. extensions, of a given symmetric operator $\hat{f}$, we can assume without loss of generality that the initial

[10]Another name, probably obsolete, is Hermitian operator.

symmetric operator is closed, which is usually adopted in the mathematical literature. But in physics, a preliminary symmetric operator $\hat{f}$, a "candidate to an observable", usually appears to be nonclosed, while constructing and describing the closure $\overline{\hat{f}}$ of $\hat{f}$ is generally nontrivial. In what follows, we therefore consider an initial symmetric operator $\hat{f}$ in general nonclosed. If $\hat{f}$ is, or appears, closed, the statements that follow are easily modified or simplified in an obvious way.

In general, the adjoint of a symmetric operator $\hat{f}$ is nonsymmetric, but if $\hat{f}^+$ is symmetric, then it is s.a. as well as the closure $\overline{\hat{f}}$ because $\hat{f}^+ \subseteq \left(\hat{f}^+\right)^+$ implies the inclusions $\hat{f}^+ = \overline{\hat{f}}^+ \subseteq \overline{\hat{f}} = \left(\hat{f}^+\right)^+$ inverse to the previous ones. Such a symmetric operator, i.e., a symmetric operator whose closure is s.a., is called an essentially s.a. operator. A unique s.a. extension of an essentially s.a. operator $\hat{f}$ is its closure $\overline{\hat{f}}$ that coincides with its adjoint $\hat{f}^+$. This is certainly the case if $\hat{f}$ is bounded, then we have $D_{\overline{f}} = \mathcal{H}$.

In what follows, by a symmetric operator we mean an unbounded symmetric operator.

If $\hat{f}_{\text{ext}}$ is a symmetric extension of a symmetric operator $\hat{f}$, then the chain of inclusions, $\hat{f} \subseteq \hat{f}_{\text{ext}} \subseteq \left(\hat{f}_{\text{ext}}\right)^+ \subseteq \hat{f}^+$ holds, i.e., any symmetric extension of $\hat{f}$ is a symmetric restriction of $\hat{f}^+$. This is one of the basic starting points of the theory to follow: when a symmetric operator is extended symmetrically, its extensions and their adjoints go to meet each other; if the meeting occurs, we get a s.a. operator, but the meeting may be impossible, and if possible, there may be a nonunique way for it. The problem of the theory is to describe all the possibilities.

The closure $\overline{\hat{f}}$ is a minimum closed symmetric extension of a nonclosed symmetric operator $\hat{f}$: $\overline{\hat{f}}$ is contained in any closed symmetric extension of $\hat{f}$. For brevity, we call $\overline{\hat{f}}$ the trivial symmetric extension of the a symmetric operator $\hat{f}$; if $\hat{f}_{\text{ext}}$ contains the closure $\overline{\hat{f}}$ and is different from it, $\overline{\hat{f}} \subset \hat{f}_{\text{ext}}$ (a strict inclusion), we call such an extension nontrivial.

A closed symmetric operator $\hat{f}$, $\hat{f} = \overline{\hat{f}}$, is called maximal, if it does not allow nontrivial symmetric extensions. Any s.a. operator $\hat{f}$, $\hat{f} = \hat{f}^+$, is a maximal symmetric operator.

Because we consider in general nonclosed symmetric operators, it is natural to introduce a notion of an essentially maximal operator, similarly to the notion of an essentially s.a. operator, as a symmetric operator $\hat{f}$ whose closure $\overline{\hat{f}}$ is a maximal operator, or simply, maximal.

Any symmetric operator $\hat{f}$, in particular, its closure $\overline{\hat{f}}$, can have only real eigenvalues[11], i.e., $\hat{f}\xi = \lambda\xi \Longrightarrow \lambda = \overline{\lambda}$, or

$$
\begin{gathered}
\ker\left(\hat{f} - z\hat{I}\right) = \ker\left(\overline{\hat{f}} - z\hat{I}\right) = \{0\} \ , \ \forall z \in \mathbb{C}_+ \cup \mathbb{C}_- \ , \\
\mathbb{C}_+ = \{z = x + iy : \ y > 0\} \ , \ \mathbb{C}_- = \{z = x + iy : \ y < 0\} \ .
\end{gathered}
$$

It follows that for any $z \in \mathbb{C}_+ \cup \mathbb{C}_-$, the closed operator $\overline{\hat{f}} - z\hat{I}$ is invertible and the inverse operator $\hat{R}_z = \left(\overline{\hat{f}} - z\hat{I}\right)^{-1}$ is a bounded closed operator, therefore the range $\Re_z$ of the operator $\overline{\hat{f}} - z\hat{I}$,

$$
\Re_z = R_{\bar{f}-zI} = \left\{\underline{\eta} = \left(\overline{\hat{f}} - z\hat{I}\right)\underline{\xi}\,,\ \forall\underline{\xi} \in D_{\overline{f}}\right\} \ ,
$$

[11] A proof is a standard one; it is well known to physicists as applied to s.a. operator. We only note that a symmetric operator may have no eigenvalues, whereas its symmetric extensions can have eigenvalues.

is a closed subspace in $\mathcal{H}$ as the domain of the closed bounded operator $\hat{R}_z$.

By definition, the orthogonal complement (in $\mathcal{H}$) to the range $\Re_z$ as well as to the range R_{f-zI} of the operator $\hat{f}-z\hat{I}$, is called the deficient subspace $\aleph_z$ of a symmetric operator $\hat{f}$ corresponding to a point $z \in \mathbb{C}_+ \cup \mathbb{C}_-$,

$$\begin{aligned} \aleph_z &= \left(R_{f-zI}\right)^{\perp} = \left(R_{\bar{f}-zI}\right)^{\perp} = \left(\Re_z\right)^{\perp} \\ &= \ker\left(\hat{f}^+ - \overline{z}\hat{I}\right) = \left\{\xi_{\overline{z}} \in D_{f^+} : \ \hat{f}^+\xi_{\overline{z}} = \overline{z}\xi_{\overline{z}}\right\} . \end{aligned}$$

A deficient subspace $\aleph_z$ is a closed subspace.

It is important that the dimension of $\aleph_z$,

$$\dim \aleph_z = \begin{cases} m_+, \ z \in \mathbb{C}_- \ (\bar{z} \in \mathbb{C}_+) \ , \\ m_-, \ z \in \mathbb{C}_+ \ (\bar{z} \in \mathbb{C}_-) \ , \end{cases}$$

is independent of z in the respective domains $\mathbb{C}_-$ and $\mathbb{C}_+$; m_+ and m_- are called the deficiency indices of the operator $\hat{f}$. For a given z, we therefore distinguish the two deficient subspaces $\aleph_z$ and $\aleph_{\bar{z}} = \left\{\xi_z \in D_{f^+} : \ \hat{f}^+\xi_z = z\xi_z\right\}$, such that if $z \in \mathbb{C}_-(\mathbb{C}_+)$ then $\dim \aleph_z = m_+\,(m_-)$ while[12] $\dim \aleph_{\bar{z}} = m_-\,(m_+)$; both m_+ and m_- can be infinite, if $m_+,\ m_- = \infty$, they are considered equal, $m_+ = m_- = \infty$.

Accordingly, the decomposition

$$\mathcal{H} = \Re_z \oplus \aleph_z \tag{2}$$

holds, which means that any vector $\xi \in \mathcal{H}$ can be represented as

$$\xi = \left(\overline{\hat{f}} - z\hat{I}\right)\underline{\xi} + \xi_{\overline{z}}\,, \tag{3}$$

with some $\underline{\xi} \in D_{\overline{f}}$ and $\xi_{\overline{z}} \in \aleph_z$ that are uniquely defined by ξ. We note that for in general nonclosed operator $\hat{f}$, its closure $\overline{\hat{f}}$ enters decompositions (2) and (3).

2.3 First von Neumann theorem

This theorem provides a basic starting point in studying symmetric and s.a. extensions of symmetric operators.

Theorem 1 *(The first von Neumann theorem) For any symmetric operator $\hat{f}$, the domain D_{f^+} of its adjoint $\hat{f}^+$ is the direct sum of the three linear manifolds $D_{\overline{f}}$, $\aleph_{\bar{z}}$ and $\aleph_z$:*

$$D_{f^+} = D_{\overline{f}} + \aleph_{\bar{z}} + \aleph_z\,,\ \forall z \in \mathbb{C}_+ \cup \mathbb{C}_-\,, \tag{4}$$

where $+$ is the symbol of a direct nonorthogonal sum, such that any vector $\xi_* \in D_{f^+}$ is uniquely represented as

$$\xi_* = \underline{\xi} + \xi_z + \xi_{\overline{z}}\,, \tag{5}$$

where $\underline{\xi} \in D_{\overline{f}}$, $\xi_z \in \aleph_{\bar{z}}$, and $\xi_{\overline{z}} \in \aleph_z$, and

$$\hat{f}^+\xi_* = \overline{\hat{f}}\underline{\xi} + z\xi_z + \overline{z}\xi_{\overline{z}}\,. \tag{6}$$

[12] We point out that there exists an anticorrespondence $z \rightleftarrows \bar{z}$ between the subscript z of $\aleph_z$ and the respective eigenvalue $\bar{z}$ and the subscript of the eigenvector $\xi_{\bar{z}}$ of $\hat{f}^+$. Perhaps it would be more convenient to change the notation $\aleph_z \rightleftarrows \aleph_{\bar{z}}$; the conventional notation is due to tradition. The same is true for the subscripts of $m_\pm$ and $C_\mp$.

Formula (5) is called the first von Neumann formula, we assign the same name to formula (4).

It should be emphasized that for in general nonclosed symmetric operator $\hat{f}$, the domain $D_{\overline{f}}$ of its closure $\overline{\hat{f}}$ enters decompositions (4)-(6).

Proof. The domain $D_{\overline{f}}$ and the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ are linear manifolds belonging to D_{f^+}, therefore, a vector $\xi_* = \underline{\xi} + \xi_z + \xi_{\overline{z}}$ belongs to D_{f^+} with any $\underline{\xi} \in D_{\overline{f}}$, $\xi_z \in \aleph_{\bar{z}}$, and $\xi_{\overline{z}} \in \aleph_z$. By the definition of a direct sum of linear manifolds, it remains to show that for any vector $\xi_* \in D_{f^+}$, a unique representation (5) holds.

Let $\xi_* \in D_{f^+}$. According to (2) and (3), the vector $\left(\hat{f}^+ - z\hat{I}\right)\xi_*$, $\forall z \in \mathbb{C}_+ \cup \mathbb{C}_-$, is represented as

$$\left(\hat{f}^+ - z\hat{I}\right)\xi_* = \left(\overline{\hat{f}} - z\hat{I}\right)\underline{\xi} + (\overline{z} - z)\,\xi_{\overline{z}}\,, \tag{7}$$

with some $\underline{\xi} \in D_{\overline{f}}$ and $\xi_{\overline{z}} \in \aleph_z$ that are uniquely defined by ξ_* (the nonzero factor $\overline{z} - z$ in front of $\xi_{\overline{z}}$ is introduced for convenience). But $\overline{\hat{f}}\underline{\xi} = \hat{f}^+\underline{\xi}$ and $\overline{z}\xi_{\overline{z}} = \hat{f}^+\xi_{\overline{z}}$, and (7) becomes

$$\left(\hat{f}^+ - z\hat{I}\right)\xi_* = \left(\hat{f}^+ - z\hat{I}\right)\underline{\xi} + \left(\hat{f}^+ - z\hat{I}\right)\xi_{\overline{z}}, \text{ or } \left(\hat{f}^+ - z\hat{I}\right)\left(\xi_* - \underline{\xi} - \xi_{\overline{z}}\right) = 0\,,$$

which yields $\xi_* - \underline{\xi} - \xi_{\overline{z}} = \xi_z$, or $\xi_* = \underline{\xi} + \xi_z + \xi_{\overline{z}}$, where $\xi_z \in \aleph_{\bar{z}}$ and is evidently uniquely defined by ξ_*, $\underline{\xi}$, and $\xi_{\overline{z}}$, therefore by ξ_* alone, as well as $\underline{\xi}$ and $\xi_{\overline{z}}$. This proves representation (5) for any vector $\xi_* \in D_{f^+}$.

After this, formula (6) is evident.

We note that

i) representations (4)-(6) hold for any complex, but not real, number $z = x + iy,\ y \neq 0$;

ii) these representations are explicitly z-dependent because the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ and therefore the sum $\aleph_{\bar{z}} + \aleph_z$ depend on z, but $\dim(\aleph_{\bar{z}} + \aleph_z) = m_+ + m_-$, as well as m_+ and m_-, is independent of z[13];

iii) the sum in (4) is direct, but not orthogonal, it cannot be orthogonal, at least, because $\overline{D_{\bar{f}}} = \mathcal{H}$ and therefore $D_{\overline{f}}^{\perp} = \{0\}$.

It immediately follows from the first von Neumann theorem that a nonclosed symmetric operator $\hat{f}$ is essentially s.a. (and a closed symmetric operator is s.a.) iff $\aleph_{\bar{z}} = \aleph_z = \{0\}$, i.e., iff its deficiency indices are equal to zero, $m_+ = m_- = 0$, because in this case, $D_{f^+} = D_{\overline{f}}$, therefore $\overline{\hat{f}} = \hat{f}^+$. In other words, the adjoint $\hat{f}^+$ is symmetric iff $m_+ = m_- = 0$.

But this theorem, namely, formulas (5) and (6), also allows estimating the "asymmetricity" of the adjoint $\hat{f}^+$ in the case where the deficiency indices m_+ and m_- are not equal to zero (one of them or both) and analyzing the possibilities of symmetric and s.a. extensions of $\hat{f}$. We now turn to this case, the case where $\max(m_+, m_-) \neq 0$.

2.4 Asymmetry forms ω_* and Δ_*

The consideration to follow is proceeding with some arbitrary, but fixed, complex number $z = x + iy,\ y \neq 0$. A choice of a specific z is a matter of convenience, all z are equivalent; in the mathematical literature, it is a tradition to take $z = i$ $(x = 0,\ y = 1)$.

[13]Although $\aleph_{\bar{z}}$ and $\aleph_z$ are closed subspaces in $\mathcal{H}$, we cannot in general assert that their direct sum $\aleph_{\bar{z}} + \aleph_z$ is also a closed subspace. The latter is always true if one of the subspaces is finite-dimensional.

We recall that by definition, a symmetric operator $\hat{f}$ is a densely defined operator, $\overline{D_f} = \mathcal{H}$, with the property (1). The criterion of symmetricity is that all diagonal matrix elements (all means) of a symmetric operator are real[14],

$$2i\,\mathrm{Im}\left(\xi, \hat{f}\xi\right) = \left(\xi, \hat{f}\xi\right) - \overline{\left(\xi, \hat{f}\xi\right)} = \left(\xi, \hat{f}\xi\right) - \left(\hat{f}\xi, \xi\right) = 0\,,\ \forall\xi \in D_f\,.$$

For this reason, it is natural to introduce two forms defined by the adjoint $\hat{f}^+$ in its domain D_{f^+} : the sesquilinear form ω_* given by

$$\omega_*\left(\eta_*, \xi_*\right) = \left(\eta_*, \hat{f}^+\xi_*\right) - \left(\hat{f}^+\eta_*, \xi_*\right)\,,\ \xi_*, \eta_* \in D_{f^+}\,, \tag{8}$$

and the quadratic form Δ_* given by

$$\Delta_*\left(\xi_*\right) = \left(\xi_*, \hat{f}^+\xi_*\right) - \left(\hat{f}^+\xi_*, \xi_*\right) = 2i\,\mathrm{Im}\left(\xi_*, \hat{f}^+\xi_*\right)\,,\ \xi_* \in D_{f^+}\,. \tag{9}$$

The form ω_* is anti-Hermitian, $\omega_*\left(\eta_*, \xi_*\right) = -\overline{\omega_*\left(\xi_*, \eta_*\right)}$, and the form Δ_* is pure imaginary $\overline{\Delta_*\left(\xi_*\right)} = -\Delta_*\left(\xi_*\right)$. The forms ω_* and Δ_* determine each other. Really, Δ_* is an evident restriction of ω_* to the diagonal $\xi_* = \eta_*$,

$$\Delta_*\left(\xi_*\right) = \omega_*\left(\xi_*, \xi_*\right)\,,$$

while ω_* is completely determined by Δ_* in view of the equality

$$\omega_*\left(\eta_*, \xi_*\right) = \frac{1}{4}\left\{\left[\Delta_*\left(\xi_* + \eta_*\right) - \Delta_*\left(\xi_* - \eta_*\right)\right] - i\left[\Delta_*\left(\xi_* + i\eta_*\right) - \Delta_*\left(\xi_* - i\eta_*\right)\right]\right\}$$

(the so-called polarization formula).

Each of these forms is a measure of asymmetricity of the adjoint $\hat{f}^+$, i.e., a measure of to what extent the adjoint $\hat{f}^+$ is nonsymmetric. We therefore call ω_* and Δ_* the respective sesquilinear asymmetry form and quadratic asymmetry form. If $\omega_* \equiv 0$, or equivalently $\Delta_* \equiv 0$, the adjoint $\hat{f}^+$ is symmetric and $\hat{f}$ is essentially s.a. .

2.5 Closure of symmetric operator in terms of asymmetry form ω_*

One of the immediate advantages of introducing the sesquilinear form ω_* is that it allows simply determining the closure $\overline{\hat{f}}$ of an initial generally nonclosed symmetric operator $\hat{f}$ if the adjoint $\hat{f}^+$ is determined. Really, we know that $\overline{\hat{f}}$ is symmetric, $\overline{\hat{f}} \subseteq \left(\overline{\hat{f}}\right)^+$ with the same adjoint, $\left(\overline{\hat{f}}\right)^+ = \hat{f}^+$, and coincides with the adjoint to the adjoint $\left(\hat{f}^+\right)^+$, such that $\overline{\hat{f}} = \left(\hat{f}^+\right)^+ \subseteq \left(\overline{\hat{f}}\right)^+ = \hat{f}^+$, therefore, $\overline{\hat{f}}$ can be determined as $\left(\hat{f}^+\right)^+$. The defining equation for $\left(\hat{f}^+\right)^+ = \overline{\hat{f}}$, i.e., for a pair $\underline{\psi} \in D_{\bar{f}}$ and $\underline{\chi} = \overline{\hat{f}}\underline{\psi}$, is[15]

$$\left(\underline{\psi}, \hat{f}^+\xi_*\right) - \left(\underline{\chi}, \xi_*\right) = 0\,,\ \forall\xi_* \in D_{f^+}\,. \tag{10}$$

[14] It is well known to physicists as applied to s.a. operators.

[15] Here, we use the notation $\underline{\psi}$ and $\underline{\chi}$ instead of the conventional $\underline{\xi}$ and $\underline{\eta}$ in oder to avoid a possible confusion: $\underline{\xi}$ is also a conventional notation for the $D_{\bar{f}}$-component of ξ_* in representation (5) that is used below.

But $\overline{\hat{f}} \subseteq \hat{f}^{+}$ means that $D_{\bar{f}} \subseteq D_{f^+}$, i.e., $\underline{\psi} \in D_{f^+}$, and $\underline{\chi} = \overline{\hat{f}}\underline{\psi} = \hat{f}^{+}\underline{\psi}$ (we know the "rule" for $\overline{\hat{f}}$), therefore, defining equation (10) for the closure $\overline{\hat{f}}$ reduces to the equation $\left(\underline{\psi}, \hat{f}^{+}\xi_{*}\right) - \left(\hat{f}^{+}\underline{\psi}, \xi_{*}\right) = 0\,,\ \forall \xi_{*} \in D_{f^+}$, i.e., to the equation

$$\omega_{*}\left(\underline{\psi}, \xi_{*}\right) = 0\,,\ \forall \xi_{*} \in D_{f^+}\,, \tag{11}$$

for $\underline{\psi} \in D_{\bar{f}}$ only, or equivalently, taking the complex conjugation of (11), to

$$\omega_{*}\left(\xi_{*}, \underline{\psi}\right) = 0\,,\ \forall \xi_{*} \in D_{f^+}\,, \tag{12}$$

which is the linear equation for the domain $D_{\bar{f}} \subseteq D_{f^+}$ of the closure.

The closure $\overline{\hat{f}}$ of a symmetric operator $\hat{f}$, $\hat{f} \subseteq \hat{f}^{+}$, is thus given by[16]

$$\overline{\hat{f}}: \begin{cases} D_{\bar{f}} = \left\{\underline{\psi} \in D_{f^+} : \omega_{*}\left(\xi_{*}, \underline{\psi}\right) = 0\,,\ \forall \xi_{*} \in D_{f^+}\right\}\,, \\ \overline{\hat{f}}\underline{\psi} = \hat{f}^{+}\underline{\psi}\,. \end{cases} \tag{13}$$

Formula (13) specifies the closure $\overline{\hat{f}}$ as an evidently symmetric restriction of the adjoint $\hat{f}^{+}$: $\omega_{*}\left(\xi_{*}, \underline{\psi}\right) = 0$ implies

$$\omega_{*}\left(\underline{\eta}, \underline{\xi}\right) = \left(\underline{\eta}, \overline{\hat{f}}\underline{\xi}\right) - \left(\overline{\hat{f}}\underline{\eta}, \underline{\xi}\right) = 0\,,\ \forall \underline{\eta}, \underline{\xi} \in D_{f^+}\,,$$

which confirms the fact that the closure of a symmetric operator is symmetric.

Because ω_{*} vanishes on $D_{\bar{f}}$ and because of representation (5) for $\xi_{*} \in D_{f^+}$, the nontrivial content of eq. (12) for the domain $D_{\bar{f}}$ in (13) is only due to the presence of the deficient subspaces. Really, substituting representation (5) for ξ_{*}, $\xi_{*} = \underline{\xi} + \xi_{z} + \xi_{\overline{z}}$ in (12), and using the fact that ω_{*} vanishes on $D_{\bar{f}}$, we reduce it to the equation

$$\omega_{*}\left(\xi_{z} + \xi_{\overline{z}}, \underline{\psi}\right) = 0\,,\ \forall \xi_{z} \in \aleph_{\bar{z}}\,,\ \forall \xi_{\bar{z}} \in \aleph_{z}\,, \tag{14}$$

which is equivalent to the set of equations

$$\omega_{*}\left(\xi_{z}, \underline{\psi}\right) = 0\,,\ \omega_{*}\left(\xi_{\overline{z}}, \underline{\psi}\right) = 0\,,\ \forall \xi_{z} \in \aleph_{\bar{z}}\,,\ \forall \xi_{\bar{z}} \in \aleph_{z}\,.$$

Let the deficient subspaces be finite-dimensional, $\dim \aleph_{\bar{z}} = m_{\bar{z}} < \infty$ and $\dim \aleph_{z} = m_{z} < \infty$ ($m_{\bar{z}}$ is equal to m_{+} or m_{-} and $m_{z} = m_{-}$ or m_{+} for the respective $z \in \mathbb{C}_{-}$ or $z \in \mathbb{C}_{+}$), and let $\{e_{z,k}\}_{1}^{m_{\bar{z}}}$ and $\{e_{\bar{z},k}\}_{1}^{m_{z}}$ be some basises in the respective $\aleph_{\bar{z}}$ and $\aleph_{z}$. Then the last set of equations can be replaced by a finite set

$$\omega_{*}\left(e_{z,k}, \underline{\psi}\right) = 0\,,\ \omega_{*}\left(e_{\bar{z},l}, \underline{\psi}\right) = 0\,,\ k = 1, ..., m_{\bar{z}}\,,\ l = 1, ..., m_{z}\,.$$

Taking all this into account, we can effectively replace eq. (13) specifying the closure $\hat{f}$ by

$$\overline{\hat{f}}: \begin{cases} D_{\bar{f}} = \left\{\underline{\psi} \in D_{f^+} : \omega_{*}\left(\xi_{z}, \underline{\psi}\right) = \omega_{*}\left(\xi_{\overline{z}}, \underline{\psi}\right) = 0,\ \forall \xi_{z} \in \aleph_{\bar{z}}\,,\ \forall \xi_{\bar{z}} \in \aleph_{z}\right\}\,, \\ \overline{\hat{f}}\underline{\psi} = \hat{f}^{+}\underline{\psi}\,, \end{cases} \tag{15}$$

which in the case of finite-dimensional deficient subspaces is equivalent to

$$\overline{\hat{f}}: \begin{cases} D_{\bar{f}} = \left\{\underline{\psi} \in D_{f^+} : \omega_{*}\left(e_{z,k}, \underline{\psi}\right) = \omega_{*}\left(e_{\bar{z},l}, \underline{\psi}\right) = 0,\ k = 1, ..., m_{\bar{z}}\,,\ l = 1, ..., m_{z}\right\}\,, \\ \overline{\hat{f}}\underline{\psi} = \hat{f}^{+}\underline{\psi}\,, \end{cases} \tag{16}$$

where $\{e_{z,k}\}_{1}^{m_{\bar{z}}}$ and $\{e_{\bar{z},k}\}_{1}^{m_{z}}$ are some basises in the respective deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_{z}$.

[16] We adopt this form of representing operators; it actually represents the graph of an operator.

2.6 Von Neumann formula. Symmetric extensions. Second von Neumann Theorem.

But the main blessing of the two asymmetry forms ω_* and Δ_* is that they allow effectively studying the possibilities of describing symmetric and s.a. extensions of symmetric operators. The key ideas formulated, so to say, in advance are as follows. Any symmetric extension of a symmetric operator $\hat{f}$ is a restriction of its adjoint $\hat{f}^+$ to a subdomain in D_{f^+} such that the restriction of ω_* and Δ_* to this subdomain vanishes. On the other hand, ω_* allows comparatively simply evaluating the adjoint of the extension, while Δ_* allows estimating the measure of the closedness of the extension and the possibility of a further extension. S.a. extensions, if they are possible, correspond to maximum subdomains where ω_* and Δ_* vanish, maximum in the sense that a further extension to a wider domain where ω_* and Δ_* vanish is impossible.

According to the aforesaid, the both ω_* and Δ_* vanish on the domain $D_{\bar{f}} \subset D_{f^+}$ of the closure $\overline{\hat{f}} \subseteq \hat{f}^+$,

$$\omega_*\left(\underline{\eta}, \underline{\xi}\right) = 0\,,\ \forall \underline{\eta}, \underline{\xi} \in D_{\bar{f}}\,;\ \Delta_*\left(\underline{\xi}\right) = 0\,,\ \forall \underline{\xi} \in D_{\bar{f}}\,, \tag{17}$$

and are nonzero only because of the presence of the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$.

We now evaluate $\omega_*\left(\eta_*, \xi_*\right)$. According to the first von Neumann theorem 1, representation (5) holds for any $\eta_*, \xi_* \in D_{f^+}$. Substituting this representation for both η_* and ξ_* in $\omega_*\left(\eta_*, \xi_*\right)$ using the sesquilinearity of the form ω_* and taking the facts that $\omega_*\left(\underline{\eta}, \xi_*\right) = 0$, see (11), and $\omega_*\left(\eta_z + \eta_{\bar{z}}, \underline{\xi}\right) = 0$, see (14), into account, we obtain that $\omega_*\left(\eta_*, \xi_*\right) = \omega_*\left(\eta_z + \eta_{\bar{z}}, \xi_z + \xi_{\bar{z}}\right)$. Then using definition (8) of ω_* and the definition of the deficient subspaces according to which

$$\hat{f}^+\xi_z = z\xi_z\,,\ \hat{f}^+\eta_z = z\eta_z\,,\ \ \hat{f}^+\xi_{\bar{z}} = \bar{z}\xi_{\bar{z}}\,,\ \hat{f}^+\eta_{\bar{z}} = \bar{z}\eta_{\bar{z}}\,,$$

we finally find

$$\omega_*\left(\eta_*, \xi_*\right) = 2iy\left[\left(\eta_z, \xi_z\right) - \left(\eta_{\bar{z}}, \xi_{\bar{z}}\right)\right]\,,\ 2iy = \left(z - \bar{z}\right)\,. \tag{18}$$

It follows a similar representation for $\Delta_*\left(\xi_*\right) = \omega_*\left(\xi_*, \xi_*\right)$:

$$\Delta_*\left(\xi_*\right) = 2iy\left(\left\|\xi_z\right\|^2 - \left\|\xi_{\bar{z}}\right\|^2\right)\,. \tag{19}$$

Formula (19) is sometimes called the von Neumann formula (without a number).

We really see that the asymmetricity of the adjoint $\hat{f}^+$ is due to the deficient subspaces. What is more, ω_* and Δ_* are of a specific structure: up to a nonzero factor $(z - \bar{z}) = 2iy$, the contributions of the different deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ are of the opposite signs and, in principle, can compensate each other under an appropriate correspondence between ξ_z and $\xi_{\bar{z}}$, the respective $\aleph_{\bar{z}}$- and $\aleph_z$-components of vectors $\xi_* \in D_{f^+}$.

In our exposition, these formulas (18) and (19) together with the first von Neumann theorem form a basis for estimating the possibility and constructing, if possible, s.a. extensions of a symmetric operator $\hat{f}$. Although the forms ω_* and Δ_* and the respective formulas (18) and (19) are equivalent, it is convenient to use the both of them, one or another in dependence of the context.

An alternative method for studying and constructing symmetric and s.a. extensions of symmetric operators is based on the so-called Cayley transformation of a closed symmetric operator $\hat{f}$, $\hat{f} = \overline{\hat{f}}$, to an isometric operator $\hat{V} = \left(\hat{f} - z\hat{I}\right)\left(\hat{f} - \bar{z}\hat{I}\right)^{-1}$, with the domain $D_V = \Re_{\bar{z}} = R_{f - \bar{z}I}$ and the range $R_V = \Re_z = R_{f - zI}$, and vice versa, $\hat{f} = \left(z\hat{I} - \bar{z}\hat{V}\right)\left(\hat{I} - \hat{V}\right)^{-1}$; all that can be found in [7, 8].

A nontrivial symmetric extension $\hat{f}_{\text{ext}}$ of a symmetric operator $\hat{f}$, $\overline{\hat{f}} \subset \hat{f}_{\text{ext}} \subseteq \hat{f}^{+}_{\text{ext}} \subset \hat{f}^{+}$ with the domain $D_{f_{\text{ext}}}$, $D_{\bar{f}} \subset D_{f_{\text{ext}}} \subset D_{f^+}$ is possible only at the expense of deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$:

$$D_{f_{\text{ext}}} = \left\{ \xi_{\text{ext}} = \underline{\xi} + \xi_{z,\text{ext}} + \xi_{\bar{z},\text{ext}} \, , \ \forall \underline{\xi} \in D_{\bar{f}} \, , \ \xi_{z,\text{ext}} \in \aleph_{\bar{z}} \, , \ \xi_{\bar{z},\text{ext}} \in \aleph_z \right\} \, ,$$

(any $\underline{\xi} \in D_{\bar{f}}$ and some $\xi_{z,\text{ext}} \in \aleph_{\bar{z}}$ and $\xi_{\bar{z},\text{ext}} \in \aleph_z$) , or $D_{f_{\text{ext}}} = D_{\bar{f}} + \Delta D_{f_{\text{ext}}}$, where $\Delta D_{f_{\text{ext}}} = \left\{ \Delta\xi_{\text{ext}} = \xi_{z,\text{ext}} + \xi_{\bar{z},\text{ext}} \right\} \subseteq \aleph_{\bar{z}} + \aleph_z$, is nontrivial, $\Delta D_{f_{\text{ext}}} \neq \{0\}$.

$\Delta D_{f_{\text{ext}}}$ is a subspace as well as $D_{f_{\text{ext}}}$, therefore, the sets $\Delta D_{\bar{z},\text{ext}} = \{\xi_{z,\text{ext}}\} \subset \aleph_{\bar{z}}$ and $\Delta D_{z,\text{ext}} = \{\xi_{\bar{z},\text{ext}}\} \subset \aleph_z$ of the respective $\xi_{z,\text{ext}}$ and $\xi_{\bar{z},\text{ext}}$ involved must also be subspaces. We caution against that $\Delta D_{f_{\text{ext}}}$ belonging to $\aleph_{\bar{z}} + \aleph_z$ be considered a direct sum of $\Delta D_{\bar{z},\text{ext}}$ and $\Delta D_{z,\text{ext}}$, $\Delta D_{f_{\text{ext}}} \neq \Delta D_{\bar{z},\text{ext}} + \Delta D_{z,\text{ext}}$, see below.

The crucial remark is then that a symmetric extension $\hat{f}_{\text{ext}}$ of $\hat{f}$ to $D_{f_{\text{ext}}} = D_{\bar{f}} + \Delta D_{f_{\text{ext}}}$ is simultaneously a symmetric restriction of the adjoint $\hat{f}^{+}$ to $D_{f_{\text{ext}}} \subset D_{f^+}$. In particular, this implies that we know the "rule" for $\hat{f}_{\text{ext}}$: according to (6), it acts as $\overline{\hat{f}}$ on $D_{\bar{f}}$ and as a multiplication by z on $\Delta D_{\bar{z},\text{ext}}$ and by $\bar{z}$ on $\Delta D_{z,\text{ext}}$.

The requirement that the restriction $\hat{f}_{\text{ext}}$ of the adjoint $\hat{f}^{+}$ to a subspace $D_{f_{\text{ext}}} \subset D_{f^+}$ be symmetric is equivalent to the requirement that the restriction of the asymmetry forms ω_* and Δ_* to $D_{f_{\text{ext}}}$ vanish,

$$\omega_* \left(\eta_{\text{ext}}, \xi_{\text{ext}}\right) = 0, \ \forall \eta_{\text{ext}}, \xi_{\text{ext}} \in D_{f_{\text{ext}}}; \ \Delta_* \left(\xi_{\text{ext}}\right) = 0 \, , \ \forall \xi_{\text{ext}} \in D_{f_{\text{ext}}} \, . \tag{20}$$

We now establish the necessary and sufficient conditions for the existence of such nontrivial domain $D_{f_{\text{ext}}}$ and describe their structure. Each of conditions (20) is equivalent to another. In the consideration to follow, we mainly deal with the quadratic asymmetry form Δ_*.

According to von Neumann formula (19), the only nontrivial point in the condition $\Delta_* \left(\xi_{\text{ext}}\right) = 0$ is that the restriction of Δ_* to $\Delta D_{f_{\text{ext}}}$ vanishes:

$$\Delta_* \left(\Delta\xi_{\text{ext}} = \xi_{z,\text{ext}} + \xi_{\bar{z},\text{ext}}\right) = 2iy \left(\left\|\xi_{z,\text{ext}}\right\|^2 - \left\|\xi_{\bar{z},\text{ext}}\right\|^2 \right) = 0 \, , \ \forall \Delta\xi_{\text{ext}} \in \Delta D_{f_{\text{ext}}} \, . \tag{21}$$

It immediately follows that if one of the deficient subspaces of the initial symmetric operator $\hat{f}$ is trivial, i.e., if $\aleph_{\bar{z}} = \{0\}$ or $\aleph_z = \{0\}$, or, equivalently, if one of the deficiency indices is equal to zero, i.e., if $m_+ = 0$ or $m_- = 0$, in short, $\min\left(m_+, m_-\right) = 0$, then there is no nontrivial symmetric extensions of this operator. In other words, a symmetric operator $\hat{f}$ with one of the deficiency indices equal to zero, $\min\left(m_+, m_-\right) = 0$, is essentially maximal.

In what follows, we therefore consider the case where $\min\left(m_+, m_-\right) \neq 0$ and the both deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ of a symmetric operator $\hat{f}$ are nontrivial. We show that in this case, nontrivial symmetric extensions of $\hat{f}$ do exist. Without loss of generality, we assume that

$$0 < \dim \aleph_{\bar{z}} = \min\left(m_+, m_-\right) \leq \dim \aleph_z = \max\left(m_+, m_-\right) \, ,$$

we can always take an appropriate z. In the mathematical literature, it is conventional to take $z \in \mathbb{C}_+$, $y > 0$, then if $0 < m_+ \leq m_-$, we fall into our condition; in the opposite case, the deficient subspaces and deficiency indices are simply transposed in the consideration to follow.

We first assume the existence of nontrivial symmetric extensions in the case under consideration. Let $\hat{f}_{\text{ext}}$ be a nontrivial symmetric extension of a symmetric operator $\hat{f}$ with the both deficiency indices m_+ and m_- different from zero. Formula (21) suggests that the both deficient

subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ must be involved in this extension, i.e., $\Delta D_{\bar{z},\text{ext}} \neq \{0\}$ and $\Delta D_{z,\text{ext}} \neq \{0\}$, and any involved $\xi_{z,\text{ext}} \in \Delta D_{\bar{z},\text{ext}} \subseteq \aleph_{\bar{z}}$ must be assigned a certain $\xi_{\bar{z},\text{ext}} \in \Delta D_{z,\text{ext}} \subseteq \aleph_z$ of the same norm, $\left\|\xi_{z,\text{ext}}\right\| = \left\|\xi_{\bar{z},\text{ext}}\right\|$, for their contributions to Δ_* compensate each other. We now note that this assignment must be a one-to-one correspondence. Really, if, for example, a vector $\Delta\xi_{\text{ext}} = \xi_{z,\text{ext}} + \xi_{\bar{z},\text{ext}}$ and a vector $\Delta\xi'_{\text{ext}} = \xi_{z,\text{ext}} + \xi'_{\bar{z},\text{ext}}$ belong to $\Delta D_{f_{\text{ext}}}$, then their difference $\Delta\xi'_{\text{ext}} - \Delta\xi_{\text{ext}} = \xi'_{\bar{z},\text{ext}} - \xi_{\bar{z},\text{ext}}$ with the zero $\aleph_{\bar{z}}$-component also belongs to $\Delta D_{f_{\text{ext}}}$ because $\Delta D_{f_{\text{ext}}}$ is a linear manifold. But then formula (21) implies that $\left\|\xi'_{\bar{z},\text{ext}} - \xi_{\bar{z},\text{ext}}\right\| = 0$, i.e., $\xi'_{\bar{z},\text{ext}} = \xi_{\bar{z},\text{ext}}$. A similar consideration for a pair of vectors $\Delta\xi_{\text{ext}} = \xi_{z,\text{ext}} + \xi_{\bar{z},\text{ext}} \in \Delta D_{f_{\text{ext}}}$ and $\Delta\xi'_{\text{ext}} = \xi'_{z,\text{ext}} + \xi_{\bar{z},\text{ext}} \in \Delta D_{f_{\text{ext}}}$ results in the conclusion that there must be $\xi'_{z,\text{ext}} = \xi_{z,\text{ext}}$. In addition, this correspondence must be a linear mapping of $\Delta D_{\bar{z},\text{ext}}$ to $\Delta D_{z,\text{ext}}$ for $\Delta D_{f_{\text{ext}}}$ to be a linear manifold.

But this means that any nontrivial symmetric extension $\hat{f}_{\text{ext}}$ of $\hat{f}$ is defined by some linear isometric mapping, or simply isometry,

$$\hat{U} : \aleph_{\bar{z}} \longrightarrow \aleph_z ,$$

with a domain $D_U = \Delta D_{\bar{z},\text{ext}} \subseteq \aleph_{\bar{z}}$ and a range $R_U = \Delta D_{z,\text{ext}} = \hat{U}\Delta D_{\bar{z},\text{ext}} \subseteq \aleph_z$. Because any isometry preserves dimension, $\Delta D_{\bar{z},\text{ext}}$ and $\Delta D_{z,\text{ext}}$ must be of the same dimension,

$$\dim \Delta D_{\bar{z},\text{ext}} = \dim \Delta D_{z,\text{ext}} = m_U \leq \min\left(m_+, m_-\right);$$

$\Delta D_{f_{\text{ext}}}$ is also of dimension m_U because of the one-to-one correspondence between the $\xi_{\bar{z},\text{ext}}$ and $\xi_{z,\text{ext}}$ components in any vector $\Delta\xi_{\text{ext}} \in \Delta D_{f_{\text{ext}}}$.

It is now reasonable to change the notation: we let D_U denote $\Delta D_{\bar{z},\text{ext}}$ and let $\hat{U}D_U$ denote $\Delta D_{z,\text{ext}}$ and change the subscript "ext" to the subscript "U" in other cases, such that $\hat{f}_{\text{ext}}$, $D_{f_{\text{ext}}}$, $\Delta D_{f_{\text{ext}}}$, and etc. are now denoted by $\hat{f}_U$, D_{f_U}, ΔD_{f_U}, and etc. In particular, D_{f_U} is now written as

$$\begin{aligned}
&D_{f_U} = D_{\bar{f}} + \Delta D_{f_U} = \left\{\xi_U = \underline{\xi} + \Delta\xi_U ,\ \forall\underline{\xi} \in D_{\bar{f}} ,\ \forall\Delta\xi_U \in \Delta D_{f_U}\right\} ,\\
&\Delta D_{f_U} = \left(D_U + \hat{U}D_U\right) = \left(\hat{I} + \hat{U}\right) D_U = \left\{\Delta\xi_U = \xi_{z,U} + \xi_{\bar{z},U} ,\right.\\
&\left.\xi_{z,U} \in D_U \subseteq \aleph_{\bar{z}} ,\ \xi_{\bar{z},U} = \hat{U}\xi_{z,U} \in \hat{U}D_U \subseteq \aleph_z\right\} ,
\end{aligned} \tag{22}$$

where the parenthesis in the notation $\left(D_U + \hat{U}D_U\right)$ denotes that ΔD_{f_U} is not a direct sum of the linear manifolds D_U and $\hat{U}D_U$ of equal dimension $m_U \leq \min\left(m_+, m_-\right)$, but a special linear manifold of dimension m_U that can be considered a "diagonal" of the direct sum $D_U + \hat{U}D_U$.

We can now prove the existence of nontrivial symmetric extensions of a symmetric operator $\hat{f}$ in the case where $\min\left(m_+, m_-\right) \neq 0$ by reversing the above consideration. Namely, it is now evident that if the deficient subspaces of $\hat{f}$, $\aleph_{\bar{z}}$ and $\aleph_z$, are nontrivial, then any isometry $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$ with the domain $D_U \subseteq \aleph_{\bar{z}}$ and the range $\hat{U}D_U \subseteq \aleph_z$ generates a nontrivial symmetric extension $\hat{f}_U$ of $\hat{f}$ as the restriction of the adjoint $\hat{f}^+$ to the domain D_U given by (22) because this restriction is evidently symmetric. It follows in particular that if $\hat{f}$ is an essentially maximal symmetric operator, then one of its deficiency indices must be zero.

We collect all the aforesaid in a theorem.

Theorem 2 *(The second von Neumann theorem) A symmetric operator $\hat{f}$ is essentially s.a. iff its deficiency indices are equal to zero, $m_+ = m_- = 0$.*

A symmetric operator $\hat{f}$ is essentially maximal iff one of its deficiency indices is equal to zero, $\min(m_+, m_-) = 0$*; if its second deficiency index is also equal to zero, then $\hat{f}$ is essentially s.a.; if the second deficiency index is nonzero, then $\hat{f}$ is only essentially maximal and does not allow s.a. extensions.*

If the both deficiency indices of a symmetric operator $\hat{f}$ are different from zero, $\min(m_+, m_-) \neq 0$*, i.e., the both its deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ are nontrivial, then nontrivial symmetric extensions of $\hat{f}$ do exist. Any symmetric extension $\hat{f}_U$ of $\hat{f}$ is defined by some isometric operator $\hat{U}$ with a domain $D_U \subseteq \aleph_{\bar{z}}$ and a range $\hat{U}D_U \subseteq \aleph_z$ and is given by*[17]

$$D_{f_U} = D_{\underline{f}} + \left(\hat{I} + \hat{U}\right) D_U = \Big\{\xi_U = \underline{\xi} + \xi_{z,U} + \hat{U}\xi_{z,U} : \\ \forall\underline{\xi} \in D_{\bar{f}}\,,\ \forall\xi_{z,U} \in D_U \subseteq \aleph_{\bar{z}}\,,\ \hat{U}\xi_{z,U} \in \hat{U}D_U \subseteq \aleph_z\Big\}\,, \tag{23}$$

and

$$\hat{f}_U\xi_U = \overline{\hat{f}}\underline{\xi} + z\xi_{z,U} + \bar{z}\hat{U}\xi_{z,U}\,. \tag{24}$$

Conversely, any isometric operator $\hat{U}: \aleph_{\bar{z}} \longrightarrow \aleph_z$ with a domain $D_U \subseteq \aleph_{\bar{z}}$ and a range $\hat{U}D_U \subseteq \aleph_z$ defines a symmetric extension $\hat{f}_U$ of $\hat{f}$ given by (23) and (24).

The formula $\xi_U = \underline{\xi} + \xi_{z,U} + \hat{U}\xi_{z,U}$ in (23) is called the second von Neumann formula.

We do not dwell on the theory of symmetric extensions of symmetric operators in every detail because it hardly can find applications in constructing quantum-mechanical observables and restrict ourselves to a few remarks on the general properties of arbitrary symmetric extensions. All the details can be found in [7, 8].

i) It is evident that if $\hat{f}_U$ is a closed extension of a symmetric operator $\hat{f}$, then D_U and $\hat{U}D_U$ are closed subspaces in the respective deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ and vice versa.

ii) The deficient subspaces of an extension $\hat{f}_U$ are the respective subspaces $\aleph_{\bar{z},U} = D_U^{\perp} = \aleph_{\bar{z}} \backslash \overline{D_U}$ and $\aleph_{z,U} = \left(\hat{U}D_U\right)^{\perp} = \aleph_z \backslash \overline{\hat{U}D_U}$, the orthogonal complements of D_U and $\hat{U}D_U$ in the respective deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ of the initial symmetric operator $\hat{f}$, therefore, the deficiency indices of the extension $\hat{f}_U$ are the respective $m_{+,U} = m_+ - m_U$ and $m_{-,U} = m_- - m_U$, where $m_U = \dim D_U$. The evaluation of the deficient subspaces and deficiency indices in the particular case of a maximal symmetric extension $\hat{f}_U$ is given below. Its modification for the general case is evident.

iii) Any symmetric operator $\hat{f}$ with the both deficiency indices different from zero can be extended to a maximal symmetric operator, see below.

iv) The description of symmetric extensions of a symmetric operator $\hat{f}$ in terms of isometries $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$ is evidently z-dependent: for a given and fixed symmetric extension of $\hat{f}$, the corresponding isometry $\hat{U}$ changes with changing z together with the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$.

2.7 Self-adjoint extensions. Main Theorem.

Our main interest here is with a possibility and a construction of s.a. extensions of symmetric operators with nonzero deficiency indices.

[17] In this case, it seems more expressive to represent the graph of the operator $\hat{f}_U$ by separate formulas.

We first note that any s.a. extension, if at all possible, is a maximal symmetric operator. This implies (in our case where $\dim \aleph_{\bar{z}} \leq \dim \aleph_z$) that the deficient subspace $\aleph_{\bar{z}}$ must be involved in the extension as a whole, i.e., $D_U = \aleph_{\bar{z}}$, otherwise, a further symmetric extension is possible by extending the isometry $\hat{U}$ to the whole $\aleph_{\bar{z}}$. The domain of a maximal symmetric extension $\hat{f}_U$ of $\hat{f}$ is thus given by

$$\begin{aligned} D_{f_U} &= D_{\overline{f}} + \left(\hat{I} + \hat{U}\right) \aleph_{\bar{z}} \\ &= \left\{ \xi_U = \underline{\xi} + \xi_z + \hat{U}\xi_z : \forall \underline{\xi} \in D_{\bar{f}} \,,\ \forall \xi_z \in \aleph_{\bar{z}} \,,\ \hat{U}\xi_z \in \aleph_z \right\} , \end{aligned} \tag{25}$$

while $\aleph_z$ can be represented as $\aleph_z = \hat{U}\aleph_{\bar{z}} \oplus \left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$, where

$$\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} = \left\{ \xi_{\bar{z},U}^{\perp} \in \aleph_z : \left(\xi_{\bar{z},U}^{\perp}, \hat{U}\xi_z\right) = 0 \,,\ \forall \xi_z \in \aleph_{\bar{z}} \right\}$$

is the orthogonal complement of a subspace $\hat{U}\aleph_{\bar{z}} \subseteq \aleph_z$ in the deficient subspace $\aleph_z$.

We now evaluate the adjoint $\hat{f}_U^+$. Because both $\hat{f}_U$ and $\hat{f}_U^+$ are the restrictions of the adjoint $\hat{f}^+$, $\hat{f}_U \subseteq \hat{f}_U^+ \subset \hat{f}^+$, we can use arguments similar to those in evaluating the closure $\overline{\hat{f}}$ of $\hat{f}$, see formulas (10)-(13): the defining equation for $\hat{f}_U^+$ is reduced to a linear equation for a domain $D_{f_U^+} \subset D_{f^+}$, i.e., for vectors $\eta_{*U} \in D_{f_U^+}$, namely,

$$\omega_* \left(\xi_U, \eta_{*U}\right) = 0 \,,\ \forall \xi_U \in D_{f_U} \,. \tag{26}$$

Let $\eta_{*U} = \underline{\eta} + \eta_z + \eta_{\bar{z}}$ be representation (5) for η_{*U}, which we rewrite as

$$\eta_{*U} = \underline{\eta} + \eta_z + \hat{U}\eta_z + \left(\eta_{\bar{z}} - \hat{U}\eta_z\right) = \eta_U + \left(\eta_{\bar{z}} - \hat{U}\eta_z\right) ,$$

where $\eta_U \in D_{f_U}$, see (25), and $\eta_{\bar{z}} - \hat{U}\eta_z \in \aleph_z$. Because ω_* vanishes on D_{f_U}, see (20), equation (26) reduces to the equation for the component $\eta_{\bar{z}} - \hat{U}\eta_z \in \aleph_z$,

$$\omega_* \left(\xi_U, \eta_{\bar{z}} - \hat{U}\eta_z\right) = 0 \,,\ \forall \xi_U \in D_{f_U} \,.$$

Substituting now representation (25) for ξ_U, $\xi_U = \underline{\xi} + \xi_z + \hat{U}\xi_z$, and using representation (18) for ω_*, we finally obtain that $(\hat{U}\xi_z, \eta_{\bar{z}} - \hat{U}\eta_z) = 0 \,,\ \forall \xi_z \in \aleph_{\bar{z}}$, which implies that $\eta_{\bar{z}} - \hat{U}\eta_z = \eta_{\bar{z},U}^{\perp} \in \left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$. Any $\eta_{*U} \in D_{f_U^+}$ is thus represented as

$$\eta_{*U} = \eta_U + \eta_{\bar{z},U}^{\perp} \,, \tag{27}$$

with some $\eta_U \in D_{f_U}$ and some $\eta_{\bar{z},U}^{\perp} \in \left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} \subset \aleph_z$.

Conversely, it is evident from the above consideration that a vector η_{*U} of form (27) with any $\eta_U \in D_{f_U}$ and any $\eta_{\bar{z},U}^{\perp} \in \left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$ satisfies defining equation (26) and therefore belongs to $D_{f_U^+}$.

Naturally changing the notation $\eta_{*U} \to \xi_{*U}$, we thus obtain that

$$D_{f_U^+} = D_{f_U} + \left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} = \left\{ \xi_{*U} = \xi_U + \xi_{\bar{z},U}^{\perp} \,,\ \forall \xi_U \in D_{f_U} \,,\ \forall \xi_{\bar{z},U}^{\perp} \in \left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} \right\}$$

and $\hat{f}_U^+ \xi_{*U} = \hat{f}_U \xi_U + \bar{z} \xi_{\bar{z},U}^{\perp}$.

This result allows answering the main question about possible s.a. extensions of symmetric operators. If the subspace $\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$ is nontrivial, $\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} = \aleph_z \backslash \hat{U}\aleph_{\bar{z}} \neq \{0\}$, we have the strict inclusion $D_{f_U} \subset D_{f_U^+}$, i.e., the extension $\hat{f}_U$ is only maximal, but not s.a., symmetric operator; if this subspace is trivial, $\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} = \{0\}$, we have $D_{f_U} = D_{f_U^+}$, which implies the equality $\hat{f}_U = \hat{f}_U^+$, i.e., the maximal extension $\hat{f}_U$ is s.a.. We now evaluate the dimension $\dim\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$ of the subspace $\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$ that is the evident criteria for $\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$ be nontrivial, $\dim\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} \neq 0$, or trivial, $\dim\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} = 0$, and respectively for a maximal symmetric extension $\hat{f}_U$ be non-s.a. or s.a.. It appears that $\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$ is essentially determined by the deficiency indices of the initial symmetric operator.

If one of the (nontrivial) deficiency indices of the initial symmetric operator $\hat{f}$ is finite, i.e., in our case, $\dim \aleph_{\bar{z}} = \min(m_+, m_-) < \infty$ (we remind that we consider the case where $\min(m_+, m_-) \neq 0$), while the other, $\dim \aleph_z = \max(m_+, m_-)$, can be infinite, then we have

$$\begin{aligned}\dim\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} &= \dim \aleph_z - \dim\left(\hat{U}\aleph_{\bar{z}}\right) = \dim \aleph_z - \dim \aleph_{\bar{z}} \\ &= \max(m_+, m_-) - \min(m_+, m_-) = |m_+ - m_-| \ ,\end{aligned}$$

where we use the equality $\dim\left(\hat{U}\aleph_{\bar{z}}\right) = \dim \aleph_{\bar{z}}$. If the both deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ are infinite dimensional, $m_+ = m_- = \infty$, we encounter the uncertainty $\dim\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} = \infty - \infty$, and a specific consideration is required. The point is that in this case, the isometry $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$ defining a maximal symmetric extension $\hat{f}_U$ can be isometric mapping of the infinite-dimensional subspace $\aleph_{\bar{z}}$ both into and onto the infinite-dimensional subspace $\aleph_z$. In the case "into", the subspace $\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$ is nontrivial, $\dim\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} \neq 0$, while in the case "onto", the subspace $\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$ is trivial, $\dim\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} = 0$.

It follows that

i) a symmetric operator $\hat{f}$ with different deficiency indices, $m_+ \neq m_-$, (which implies $\min(m_+, m_-) < \infty$) has no s.a. extensions, but only maximal symmetric extensions;

ii) a symmetric operator $\hat{f}$ with equal and finite deficiency indices, $m_+ = m_- = m < \infty$, has s.a. extensions, and what is more, any maximal symmetric extension of such an operator is s.a.;

iii) a symmetric operator $\hat{f}$ with infinite deficiency indices, $m_+ = m_- = \infty$, allows both a s.a. and non-s.a. maximal extensions.

Any s.a. extension is defined by an isometric mapping $\hat{U}$ of one of the deficient subspaces, for example, $\aleph_{\bar{z}}$, to another deficient subspace, $\aleph_z$, $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$. This mapping establishes an isomorphism between the deficient subspaces. Conversely, any such an isometric mapping $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$ defines a s.a. extension $\hat{f}_U$ of $\hat{f}$ given by (23) and (24) with $D_U = \aleph_{\bar{z}}$ and $\hat{U} D_U = \aleph_z$.

We note that there is another way (maybe, more informative) of establishing these results. It seems evident from (25) and can be proved using arguments similar to those in proving

the first von Neumann theorem that in our case, the deficient subspaces of a maximal symmetric extension $\hat{f}_U$ are $\aleph_{\bar{z},U} = \{0\}$ and $\aleph_{z,U} = \left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} \subseteq \aleph_z$ and its respective deficiency indices are $\dim \aleph_{\bar{z},U} = \min(m_{+U}, m_{-U}) = 0$ and $\dim \aleph_{z,U} = \max(m_{+U}, m_{-U}) = \dim\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$ (which confirms that $\hat{f}_U$ is really a maximal symmetric operator). It then remains to evaluate $\dim\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$ and to refer to the above-established relation between the deficiency indices of a maximal symmetric operator and its self-adjointness: a maximal symmetric operator is s.a. iff the both its deficient indices are equal to zero.

The presented consideration seems more direct.

A s.a. extension of a symmetric operator $\hat{f}$ with equal deficiency indices, i.e., with isomorphic deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$, the extension specified by an isometry $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$ and given by formulas (23) and (24) with $D_U = \aleph_{\bar{z}}$ and $\hat{U}D_U = \aleph_z$, can be equivalently defined in terms of the sesquilinear asymmetry form ω_* similarly to the closure $\overline{\hat{f}}$, see formulas (13) and (14). Namely, $\hat{f}_U$ is such an extension iff it is a restriction of the adjoint $\hat{f}^+$ to the domain D_{f_U} that is defined by the linear equation

$$\omega_*\left(\eta_z + \hat{U}\eta_z, \xi_U\right) = 0\,,\ \xi_U \in D_{f_U} \subset D_{f^+}\,,\ \forall \eta_z \in \aleph_{\bar{z}}\,. \tag{28}$$

Necessity. Let $\hat{f}_U$ be a s.a. extension of $\hat{f}$. Then the restriction of the form ω_* to its domain D_{f_U} vanishes, see (20), $\omega_*(\eta_U, \xi_U) = 0$, $\forall \xi_U, \eta_U \in D_f$. Using now the representation $\eta_U = \underline{\eta} + \eta_z + \hat{U}\eta_z$ and the equality $\omega_*\left(\underline{\eta}, \xi_U\right) = 0$, see (11) with $\underline{\psi} = \underline{\eta}$ and $\xi_* = \xi_U$, we reduce this equation to (28).

Sufficiency. Let $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$ be an isometry of one of the deficient subspaces onto another. We consider linear equation (28) for a subspace $D_{f_U} = \{\xi_U\} \subset D_{f^+}$ and show that its general solution is

$$\xi_U = \underline{\xi} + \xi_z + \hat{U}\xi_z\,,\ \forall \underline{\xi} \in D_{\bar{f}}\,,\ \forall \xi_z \in \aleph_{\bar{z}}\,,\ \hat{U}\xi_z \in \aleph_{\bar{z}}\,. \tag{29}$$

Really, a vector ξ_U of form (29) evidently satisfies eq. (28):

$$\omega_*\left(\eta_z + \hat{U}\eta_z, \underline{\xi} + \xi_z + \hat{U}\xi_z\right) = 2iy\left[(\eta_z, \xi_z) - \left(\hat{U}\eta_z, \hat{U}\xi_z\right)\right] = 0\,,$$

where we use eq. (18) and the fact that $\hat{U}$ is an isometry. Conversely, let a vector $\xi_U \in D_{f^+}$ satisfies eq. (28), then representing it as

$$\xi_U = \underline{\xi} + \xi_z + \xi_{\bar{z}} = \underline{\xi} + \xi_z + \hat{U}\xi_z + \left(\xi_{\bar{z}} - \hat{U}\xi_z\right)\,,\ \underline{\xi} \in D_{\bar{f}}\,,\ \xi_z \in \aleph_{\bar{z}}\,,\ \xi_{\bar{z}}, \hat{U}\xi_z \in \aleph_z\,,$$

and using again formulas (18) and the isometricity of $\hat{U}$, we reduce eq. (28) to $\left(\hat{U}\eta_z, \xi_{\bar{z}} - \hat{U}\xi_z\right) = 0\,,\ \forall \eta_z \in \aleph_{\bar{z}}$, whence it follows that $\xi_{\bar{z}} - \hat{U}\xi_z = 0$, or $\xi_{\bar{z}} = \hat{U}\xi_z$, because the subspace $\left\{\hat{U}\eta_z, \forall \eta_z \in \aleph_{\bar{z}}\right\} = \hat{U}\aleph_{\bar{z}} = \aleph_z$.

Actually, eq. (28) is the defining equation for the adjoint $\hat{f}_U^+$ of the operator $\hat{f}_U$ that is the restriction of the adjoint $\hat{f}^+$ to the domain $D_{f_U} = D_{\bar{f}} + \left(\hat{I} + \hat{U}\right)\aleph_{\bar{z}}$, the equation that we already encounter above, see eq. (26), where the substitutions $\xi_U \to \eta_U$ and $\eta_{*U} \to \xi_U$ must be made. Its solution in the case where $\hat{U}\aleph_{\bar{z}} = \aleph_z$ shows that $\hat{f}_U^+ = \hat{f}_U$.

In the case of a symmetric operator $\hat{f}$ with equal and finite deficiency indices, $m_+ = m_- = m < \infty$, an isometry $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$, and thereby a s.a. extension $\hat{f}_U$, can be specified by a unitary $m \times m$ matrix. For this purpose, we choose some orthobasis $\{e_{z,k}\}_1^m$ in $\aleph_{\bar{z}}$, such that any vector $\xi_z \in \aleph_{\bar{z}}$ is represented as $\xi_z = \sum_{k=1}^m c_k e_{z,k}\,,\ c_k \in \mathbb{C}\,,$ and some orthobasis $\{e_{\bar{z},l}\}_1^m$ in $\aleph_z$. Then any isometric operator $\hat{U}$ with the domain $\aleph_{\bar{z}}$ and the range $\aleph_z$ is given by

$$\hat{U} e_{z,k} = \sum_{k=1}^{m} U_{lk} e_{\bar{z},l}\,,\ \text{or}\ \hat{U}\xi_z = \sum_{l=1}^{m}\left(\sum_{k=1}^{m} U_{lk} c_k\right) e_{\bar{z},l}\,,$$

where $U = ||U_{lk}||\,,\ l,k = 1,...,m$, is a unitary matrix. Conversely, any unitary $m \times m$ matrix U defines an isometry $\hat{U}$ given by the above formulas. It is evident that for a given $\hat{U}$, the matrix U changes appropriately with the change of the orthobasises$\{e_{z,k}\}_1^m$ and $\{e_{\bar{z},l}\}_1^m$.

It follows that in the case under consideration, the family $\left\{\hat{f}_U\right\}$ of all s.a. extensions of a given symmetric operator $\hat{f}$ is a manifold of dimension m^2 that is a unitary group $U(m)$.

This result can be extended to the case of infinite deficiency indices, $m = \infty$, but with a special assignment of a meaning for the indices l and k ranging from 1 to ∞.

Because in the case where the both deficiency indices coincide, there is no difference in the choice $z \in \mathbb{C}_+$ or $z \in \mathbb{C}_-$, we take $z \in \mathbb{C}_+$, i.e., $z = x + iy,\ y > 0$, in what follows, such that from now on, $m_+ = \dim \aleph_{\bar{z}}$ and $m_- = \dim \aleph_z$.

We now summarize all the relevant previous results in a theorem. This theorem is of paramount importance: it is just what we need from mathematics for our physical purposes. We therefore present the main theorem and the subsequent comments in great detail, in fact, in an independent self-contained way for ease of using without any further references.

Theorem 3 *(The main theorem) Let $\hat{f}$ be an (in general nonclosed) symmetric operator with a domain D_f in a Hilbert space $\mathcal{H}$, $\hat{f} \subseteq \hat{f}^+$, where $\hat{f}^+$ is the adjoint, let $\aleph_{\bar{z}}$ and $\aleph_z$ be the deficient subspaces of $\hat{f}$,*

$$\aleph_{\bar{z}} = \ker\left(\hat{f}^+ - z\hat{I}\right) = \left\{\xi_z : \hat{f}^+\xi_z = z\xi_z\right\}$$

and

$$\aleph_z = \ker\left(\hat{f}^+ - \bar{z}\hat{I}\right) = \left\{\xi_{\bar{z}} : \hat{f}^+\xi_{\bar{z}} = \bar{z}\xi_{\bar{z}}\right\},$$

where z is an arbitrary, but fixed, complex number in the upper half-plane, $z = x + iy,\ y > 0$, and let m_+ and m_- be the deficiency indices of $\hat{f}$,

$$m_+ = \dim \aleph_{\bar{z}}\,,\ m_- = \dim \aleph_z\,,$$

m_+ and m_- are independent of z.

The operator $\hat{f}$ has s.a. extensions $\hat{f}_U = \hat{f}_U^+$, $\hat{f} \subseteq \hat{f}_U$, iff the both its deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ are isomorphic and are therefore of the same dimension, i.e., iff its deficiency indices m_+ and m_- are equal, $m_+ = m_- = m$.

If the deficient subspaces are trivial, $\aleph_{\bar{z}} = \aleph_z = \{0\}$, i.e., if the both deficiency indices m_+ and m_- are equal to zero, $m_+ = m_- = 0$, the operator $\hat{f}$ is essentially s.a., and its unique s.a. extension is its closure $\overline{\hat{f}} = \left(\hat{f}^+\right)^+$ which coincides with its adjoint, $\overline{\hat{f}} = \left(\overline{\hat{f}}\right)^+ = \hat{f}^+$.

If the deficient subspaces are nontrivial, i.e., if the deficiency indices are different from zero, $m \neq 0$, there exists an m^2-parameter family $\left\{\hat{f}_U\right\}$ of s.a. extensions that is the manifold $U(m)$, the unitary group.

Each s.a. extension $\hat{f}_U$ is defined by an isometric mapping $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$ of one of the deficient subspaces onto another, which establishes an isomorphism between the deficient subspaces, and is given by

$$D_{f_U} = D_{\bar{f}} + \left(\hat{I} + \hat{U}\right) \aleph_{\bar{z}} = \left\{\xi_U = \underline{\xi} + \xi_z + \hat{U}\xi_z, \forall \underline{\xi} \in D_{\bar{f}},\ \forall \xi_z \in \aleph_{\bar{z}},\ \hat{U}\xi_z \in \aleph_z\right\} \tag{30}$$

where $D_{\bar{f}}$ is the domain of the closure $\overline{\hat{f}}$, and

$$\hat{f}_U \xi_U = \overline{\hat{f}}\underline{\xi} + z\xi_z + \bar{z}\hat{U}\xi_z\,. \tag{31}$$

Conversely, any isometry $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$ that establishes an isomorphism between the deficient subspaces defines a s.a. extension $\hat{f}_U$ of $\hat{f}$ given by (30) and (31).

The s.a. extension $\hat{f}_U$ can be equivalently defined as a s.a. restriction of the adjoint $\hat{f}^+$:

$$\hat{f}_U : \left\{ \begin{array}{l} D_{f_U} = \left\{\xi_U \in D_{f^+}\ :\ \omega_* \left(\eta_z + \hat{U}\eta_z, \xi_U\right) = 0\,,\ \forall \eta_z \in \aleph_{\bar{z}}\right\}\,, \\ \hat{f}_U \xi_U = \hat{f}^+ \xi_U\,. \end{array} \right. \tag{32}$$

If the deficient subspaces are finite-dimensional, i.e., if the deficiency indices of $\hat{f}$ are finite, $0 < m < \infty$, the s.a. extensions $\hat{f}_U$ are specified in terms of unitary matrices $U \in U(m)$. Namely, let $\{e_{z,k}\}_1^m$ and $\{e_{\bar{z},l}\}_1^m$ be some orthobasises in the respective deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$, then a s.a. extension $\hat{f}_U$ is defined by

$$D_{f_U} = \left\{\xi_U = \underline{\xi} + \sum_{k=1}^m c_k \left(e_{z,k} + \sum_{l=1}^m U_{lk} e_{\bar{z},l}\right)\,,\ \forall \underline{\xi} \in D_{\bar{f}}\,,\ \forall c_k \in \mathbb{C}\right\}\,, \tag{33}$$

and

$$\hat{f}_U \xi_U = \overline{\hat{f}}\underline{\xi} + \sum_{k=1}^m c_k \left(z e_{z,k} + \bar{z} \sum_{l=1}^m U_{lk} e_{\bar{z},l}\right)\,, \tag{34}$$

where $U = \|U_{lk}\|$, $l, k = 1, ..., m$, is a unitary matrix.

The equivalent definition of $\hat{f}_U$ in terms of the adjoint $\hat{f}^+$ becomes

$$\hat{f}_U\ : \left\{ \begin{array}{l} D_{f_U} = \{\xi_U \subset D_{f^+} : \omega_* \left(e_{z,k} + \sum_{l=1}^m U_{lk} e_{\bar{z},l}, \xi_U\right) = 0,\ k = 1, ..., m\}\,, \\ \hat{f}_U \xi_U = \hat{f}^+ \xi_U\,. \end{array} \right. \,, \tag{35}$$

Theorem 3 finishes our exposition of the general theory of s.a. extensions of symmetric operators. However, we would like to give some comments and remarks of practical importance, without being afraid of repeating ourselves, and to end this section with some practical "instructions", following from the general theory, for a quantizing physicist.

2.8 Comments and remarks

Comment 1: In the case of finite-dimensional deficient subspaces of equal dimensions, $0 < m < \infty$, any maximal symmetric extension of a symmetric operator $\hat{f}$ is s.a., while in the case of infinite-dimensional deficient subspaces, there exists a possibility of both s.a. and maximal non-s.a. extensions.

If the deficient indices of a symmetric operator $\hat{f}$ are nonequal, then there exist no s.a. extensions of $\hat{f}$.

Comment 2: Of course, s.a. extensions can be equivalently defined in terms of isometric mappings of the deficient subspace $\aleph_z$ onto $\aleph_{\bar{z}}$. In the previous terms, they are described by isometric operators $\hat{U}^{-1}$ and matrices $U^{-1} = \|\overline{U}_{kl}\|$.

Comment 3: The isometries $\hat{U} : \aleph_{\bar{z}} \to \aleph_z$ in (30), (31), and (32) that define s.a. extensions $\hat{f}_U$ of a symmetric operator $\hat{f}$ depend on z, as well as the deficient subspaces; for a given s.a. extension, they change with changing z. The same is true for the matrix $U = \|U_{lk}\|$ in (33), (34), and (35) in the case of finite deficient indices, $0 < m < \infty$. In addition, for a given s.a. extension, this matrix changes in an obvious manner with a change of the respective basises in the deficient subspaces[18].

Comment 4: The last comment is a more extensive comment concerning a possible application of the general theory of s.a. extensions of symmetric operators to physical problems of quantization, namely, to a definition of quantum-mechanical observables as s.a. operators. We give it a form of some "instructions". They are generally applied to both quantum mechanics and quantum field theory. But here, we mainly address to the case where observables are represented by differential operators, as in nonrelativistic and relativistic quantum mechanics of particles, especially having in mind physical systems with boundaries and/or singularities of interaction (potentials) (the position of singularities can coincide with boundaries), we call such systems nontrivial systems. As to differential operators, the "instructions" to follow are of a preliminary nature; a more detailed discussion of s.a. differential operators is given in the next sec.3.

A "preliminary candidate" to an observable, supplied, for example, by the canonical quantization rules for a classical observable $f(q,p))$, is usually a formal expression like $f(\hat{q},\hat{p})$, or more specifically, a formal "differential expression"[19], $f(x, -i\hbar d/dx)$, that is "s.a." only from a purely algebraic standpoint, within a formal algebra of symbols $\hat{q} = x$ and $\hat{p} = -i\hbar d/dx$ with involution. But as we incessantly repeat, such an expression is only a "rule" and is not an operator unless its domain in an appropriate Hilbert space is indicated. As to differential expressions, in a physical literature, in particular, in many textbooks on quantum mechanics for physicists, such a differential expressions are considered a s.a. differential operator in a Hilbert space of wave functions like $L^2(a,b)$ actually with an implicit assumption that its domain is the so called "natural domain" that allows the corresponding differential operations within a given Hilbert space. But in the case of nontrivial systems, such a differential operator is not only non-s.a., but even nonsymmetric. This hidden defect can manifest itself when we proceed to the eigenvalue problem. "Thus, with sufficiently singular potentials, the customary methods of finding energy eigenvalues and eigenfunctions fail" [9]: an unexpected indefiniteness in the choice of eigenfunctions or even nonphysical complex eigenvalues can occur. The early history of quantum mechanics knows such examples [10, 11, 12], which first led to the apprehension that singular potentials " do not fall into the formal structure of the Schrödinger equation and its conventional interpretation" [9]. It was later realized that some additional requirements on the wave functions are needed, for example in the form of specific boundary conditions.

The main mathematical and quantum-mechanical problem is to construct a really s.a. operator in an appropriate Hilbert space starting from a preliminary formally s.a. algebraic ex-

[18] We emphasize once again that any s.a. extension is contained in the family of s.a. extensions constructed with a chosen z and certain orthobasises in $\aleph_{\bar{z}}$ and $\aleph_z$.

[19] All notions written in inverted commas are defined more precisely in the next section.

pression $f(\hat{q},\hat{p})$, in particular, differential expression $f(x,-i\hbar d/dx)$, or as we propose to speak, a s.a. operator associated with a given formal differential expression.

1. The first step.

The first step of a standard programme for solving this problem is to give the meaning of a symmetric operator $\hat{f}$ in an appropriate Hilbert space $\mathcal{H}$ to the formal expression by indicating its domain $D_f \subseteq \mathcal{H}$ which must be dense, $\overline{D_f} = \mathcal{H}$. In the case of differential expressions and nontrivial systems, this is usually achieved by choosing a domain D_f in a Hilbert space of functions (wave functions in the conventional physical terminology) like $L^2(a,b)$ such that it avoids the problems associated with boundaries and singularities by the requirement that wave functions in D_f vanish fast enough near the boundaries and singularities. The symmetricity of $\hat{f}$ is then easily verified by integrating by parts.

2. The second step.

We then must evaluate the adjoint $\hat{f}^+$, i.e., to find its "rule" and its domain $D_{f^+} \supseteq D_f$, solving the defining equation for $\hat{f}^+$. Generally, this is a nontrivial task. Fortunately, as to differential operators, the solution for a rather general symmetric operators is known in the mathematical literature, see, for example, [6, 8, 7, 13, 14]. It usually appears that the "rule" for $\hat{f}^+$ does not change and is given by the same differential expression[20] $f(x,-i\hbar d/dx)$, but its domain is larger and is a natural domain, such that $\hat{f}^+$ is a real extension of the initial symmetric operator, $\hat{f} \subset \hat{f}^+$, the extension that is generally nonsymmetric.

3. The third step.

This step consists in evaluating the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ with some fixed $z = x+iy$, $y > 0$, as the sets of solutions of the respective (differential) equations $\hat{f}^+\xi_z = z\xi_z$, $\xi_z \in D_{f^+}$, and $\hat{f}^+\xi_{\bar{z}} = \bar{z}\xi_{\bar{z}}$, $\xi_{\bar{z}} \in D_{f^+}$, and determining the deficiency indices $m_+ = \dim \aleph_{\bar{z}}$ and $m_- = \dim \aleph_z$. This problem can also present a labour-intensive task, in the case of differential operators, it usually requires an extensive experience in special functions.

An important remark here is in order. As we already mentioned above, in the mathematical literature, there is a tradition to take $z = i$ and $\bar{z} = -i$ (we remind a reader that all $z \in \mathbb{C}_+$ (or $z \in \mathbb{C}_-$) are equivalent). But in physics, a preliminary symmetric operator $\hat{f}$ and its adjoint $\hat{f}^+$ are usually assigned a certain dimension[21]. Therefore, it is natural to choose $z = \kappa i$ and $\bar{z} = -\kappa i$, where κ is an arbitrary, but fixed, constant parameter of the corresponding dimension. In constructing a physical observable as s.a. extension of a preliminary symmetric operators $\hat{f}$, this dimensional parameter enters the theory. In particular, if preliminarily a theory has no dimensional parameter that defines a scale, a naive scale invariance of the theory can be broken after a specification of the observable.

Let the deficiency indices be found. If the deficiency indices appear unequal, $m_+ \neq m_-$, our work stops with the conclusion that there is no quantum-mechanical analogue for the given classical observable $f(q,p)$. Such a situation, nonequal deficiency indices, is encountered in physics thus preventing some classical observables to be transferred to the quantum level (an example is the momentum operator for a particle on a semi-axis, see below). We note in advance that for differential operators with real coefficients, the deficiency indices are always equal.

If the deficiency indices appear to be zero, $m_+ = m_- = 0$, our work also stops: an operator $\hat{f}$ is essentially s.a. and a uniquely defined quantum-mechanical observable is its closure $\overline{\hat{f}}$ that coincides with the adjoint $\hat{f}^+$, $\overline{\hat{f}} = \hat{f}^+$.

[20] An exception is provided by δ-like potentials.

[21] In conventional units, a certain degree of length or momentum (or energy).

If the deficiency indices appear to be equal and nonzero, $m_+ = m_- = m > 0$, the fourth step follows.

4. The fourth step.

At this step, we correctly specify all the m^2-parameter family $\left\{\hat{f}_U\right\}$ of s.a. extensions $\hat{f}_U$ of $\hat{f}$ in terms of isometries $\hat{U} : \aleph_{-i\kappa} \to \aleph_{i\kappa}$ or in terms of unitary matrices $U = \|U_{lk}\|$, $l, k = 1, \ldots, m$. The general theory provides the two ways of specification given by the main theorem. The specification based on formulas (30) and (31), or (33) and (34) (and usually presented in the mathematical literature) seems more explicit in comparison with the specification based on formulas (32) or (35), which requires solving the corresponding linear equation for the domain D_{f_U}. But the first specification assumes the knowledge of the closure $\overline{\hat{f}}$ if the initial symmetric operator is nonclosed[22], which requires solving linear equations in (13), or (15), or in (16) for the domain $D_{\bar{f}}$. The second specification can sometimes become more economical because it avoids the evaluation of the closure $\overline{\hat{f}}$ and directly deals with D_{f_U}. This specifically concerns the case of differential operators where $\hat{f}^+$ is usually given by the same differential expression as $\overline{\hat{f}}$ and where the second specification allows eventually specifying the s.a. extensions $\hat{f}_U$ in the customary form of s.a. boundary conditions. This possibility is discussed below in sec.3. We say in advance that in sec.3, we also propose the third possible way of s.a. extensions of symmetric differential operators directly in terms of, in general asymptotic, boundary conditions.

In the physical literature, there is a convention to let D_+ denote the deficient subspace $\aleph_{-i\kappa} = \ker\left(\hat{f}^+ - i\kappa\hat{I}\right)$ and let D_- denote the deficient subspace $\aleph_{i\kappa} = \ker\left(\hat{f}^+ + i\kappa\hat{I}\right)$, such that the isometry $\hat{U}$ is now written as $\hat{U} : D_+ \to D_-$. The elements of the deficient subspaces D_+ and D_- are respectively denoted by[23] ξ_+, $\hat{f}^+\xi_+ = i\kappa\xi_+$, and ξ_-, $\hat{f}^+\xi_- = -i\kappa\xi_-$, and the orthobasises in D_+ and D_- are respectively denoted by $\{e_{+,\kappa}\}^m$ and $\{e_{-,\kappa}\}^m$. In these terms, formulas (30) and (33), and formulas (31) and (34) that define a s.a. extension $\hat{f}_U$ of an initial symmetric operator $\hat{f}$ in the case of $m > 0$ become

$$
\begin{aligned}
D_{f_U} &= D_{\bar{f}} + \left(\hat{I} + \hat{U}\right) D_+ = \left\{\xi_U = \underline{\xi} + \xi_+ + \hat{U}\xi_+,\ \forall\underline{\xi} \in D_{\bar{f}},\ \forall\xi_+ \in D_+,\ \hat{U}\xi_+ \in D_-\right\} \\
&= \left\{\xi_U = \underline{\xi} + \sum_{k=1}^{m} c_k \left(e_{+,k} + \sum_{l=1}^{m} U_{lk} e_{-,l}\right),\ \forall\underline{\xi} \in D_{\bar{f}}\,,\ \forall c_k \in \mathbb{C}\right\}
\end{aligned} \tag{36}
$$

and

$$
\hat{f}_U\xi_U = \overline{\hat{f}}\underline{\xi} + i\kappa\xi_+ - i\kappa\hat{U}\xi_+ = \hat{f}\underline{\xi} + i\kappa\sum_{k=1}^{m} c_k \left(e_{+,k} - \sum_{l=1}^{m} U_{lk} e_{-,l}\right)\,,
$$

[22]We would like to stress that at this point the general theory requires evaluating the closure $\overline{\hat{f}}$, it is exactly $\overline{\hat{f}}$ and $D_{\bar{f}}$ that enter formulas (30), (31), (33), and (34), while in the physical literature, we can sometimes see that when citing and using these formulas, $\hat{f}$ and D_f stand for $\overline{\hat{f}}$ and $D_{\bar{f}}$ even for non-closed symmetric operator $\hat{f}$, which is incorrect.

[23]It is the sign in front of "i" in the latter formulas that defines the subscript $+$ or $-$ in D, see footnote 10.

while formulas (32) and (35) become

$$\hat{f}_U \,:\, \begin{cases} D_{f_U} = \left\{ \xi_U \in D_{f^+} \,:\, \omega_* \left(\xi_+ + \hat{U}\xi_+ , \xi_U \right) = 0\,,\ \forall \xi_+ \in D_+ \right\} \\ = \left\{ \xi_U \in D_{f^+} \,:\, \omega_* \left(e_{+,k} + \sum_{l=1}^{m} U_{lk} e_{-,l}\,, \xi_U \right) = 0\,,\ k = 1, ..., m \right\}\,, \\ \hat{f}_U \xi_U = \hat{f}^+ \xi_U\,. \end{cases} \tag{37}$$

At last, we should not forget that an isometry $\hat{U}$ and matrices U_{lk}, as well as D_+ and D_-, depend on the real parameter κ, and for the same s.a. extension, they change with changing κ.

There is a slightly modified method of finding s.a. operators associated with formally s.a. differential expressions $f(x, -i\hbar d/dx)$, see [7, 8]. This method differs from the above-described one by some transpositions of steps 1 and 2 and partly of steps 3 and 4 . We actually can start with the end of step 2, namely with an operator $\hat{f}^*$ given by the initial differential expression $\check{f}$ and defined in $L^2\left(a,b\right)$ on a subspace of all functions $\psi_*\left(x\right)$ such that $\left(f(x,-i\hbar d/dx)\psi_*\right)(x)$ also belongs to $L^2\left(a,b\right)$. This is the most wide "natural" domain for such an operator. The operator $\hat{f}^*$ is generally non-s.a. and even nonsymmetric. Then we evaluate its adjoint $\left(\hat{f}^*\right)^+ = \hat{f}$ and find that $\hat{f}$ is symmetric and that $\hat{f}^*$ is really the adjoint of $\hat{f}$, $\hat{f}^+ = \hat{f}^*$. It follows that $\hat{f}$ is a closed symmetric operator. After this, we can proceed to the steps 3-5.

The method was far developed for a wide class of differential operators, especially for ordinary even-order differential operators with real coefficients. Unfortunately, arbitrary odd-order or mixed deferential operators practically remained apart (see, however [15, 16]). In addition, this method is inapplicable to the physically interesting case where the coefficient functions of a differential expression f are singular at the inner points of the interval (a,b), an example is a δ-like potential, whereas the first method does work in this case.

This method is rather a method of s.a. restrictions of an initial most widely defined differential operator that is generally nonsymmetric, and all the more s.a., than the method of s.a. extensions of an initial symmetric operator. We note that, in fact, the conventional practice in physics implicitly follow this method, but, so to say, in an "extreme" form. Namely, a s.a. differential expression is considered a s.a. operator in appropriate Hilbert space of functions with implicitly assuming that its domain is the most wide natural domain. Therefore, the standard physical practice is to directly proceed to finding its spectrum and eigenfunctions as the solutions of the eigenvalue problem for the corresponding differential equation. Sometimes, this approach works: the only requirements of the square-integrability of eigenfunctions or their "normalization to δ-function" appears sufficient. From the mathematical standpoint, this means that the operator under consideration is really s.a., or from the standpoint of the first method, that an initial symmetric operator is essentially s.a.. To be true, it sometimes appears that some additional specific boundary conditions or conditions near the singularities of the potential on the wave functions are necessary for fixing the eigenfunctions. In some cases, these boundary conditions are so natural that are considered unique although this is not true. But in some cases, it appears that there is no evident way of choosing between different possibilities, and this becomes a problem for the quantum-mechanical treatment of the corresponding physical system. From the mathematical standpoint, such a situation means that the initial operator is nonsymmetric, or, from the standpoint of the first method, that an initial symmetric operator is not essentially s.a. and allows different s.a. extensions, if these are at all possible, and there is no physical arguments in favor of a certain choice.

We return to this subject once more in the next section devoted to differential operators.

5. The final step.

The final step is the standard spectral analysis, i.e., finding the spectrum and eigenvectors of the obtained s.a. extensions $\hat{f}_U$ and their proper physical interpretation, in particular, the explanation of the possible origin and the physical meaning of the new m^2 parameters associated with the isometries $\hat{U}$, or unitary matrices $U = ||U_{lk}||$, in the case where the deficiency indices are different from zero. The problem of the physical interpretation of these additional parameters that are absent in the initial formal (differential) expression f and in the initial symmetric operator $\hat{f}$ is sometimes a most difficult one. The usual attempts to solve this problem are related to the search for an appropriate regularization of singularities in f and a change of boundaries by finite walls.

The most ambitious programme is to change the initial singular (differential) expression f by a regular expression f_{reg} with m^2 parameters of regularization, such that the initial symmetric operator $\hat{f}_{\text{reg}}$ is essentially s.a., and then reproduce all the s.a. extensions $\hat{f}_U$ of a singular problem as a certain limit of the regularized s.a. operator under properly removing the regularization. This procedure is like a well-known renormalization procedure in QFT, and the new m^2 parameters may be associated with "conterterms". Of course, the regularization can be partial if some singularities and arbitrariness associated with them are well-interpreted. In many cases, this problem remains unsolved.

The above-described general procedure for constructing quantum-mechanical observables starting from preliminary formal expressions is not universally obligatory because in particular cases more direct procedures are possible, especially if there exist additional physical arguments.

For example, in some cases we can guess a proper domain D_f for initial symmetric operator $\hat{f}$ such that $\hat{f}$ appears to be essentially s.a. from the very beginning.

In other cases, it can happen that an initial symmetric operator $\hat{f}$ may be represented as $\hat{f} =$ "$\hat{a}^+$"$\hat{a} + \hat{b}$, where an operator $\hat{a}$ is densely defined and an operator "$\hat{a}^+$" is its formal "adjoint" and is also densely defined, actually, "$\hat{a}^+$" is a restriction of the really adjoint $\hat{a}^+$, and $\hat{b} = \hat{b}^+$ is a bounded operator, in particular, a constant.

There is one remarkable criterion for self-adjointness that is directly applicable to this case, we call it the Akhiezer-Glazman theorem (see [7]).

Theorem 4 *Let $\hat{a}$ be a densely defined closed operator, $\overline{D_a} = \mathcal{H}$, $\hat{a} = \overline{\hat{a}}$, therefore the adjoint $\hat{a}^+$ exists and is also densely defined. Then, the operator $\hat{f} = \hat{a}^+\hat{a}$ is s.a. , the same is true for the operator $\hat{g} = \hat{a}\hat{a}^+$.*

This theorem must seem evident for physicists by the example of the harmonic oscillator Hamiltonian. A subtlety is that $\hat{a}$ must be closed.

Based on the Akhiezer–Glazman theorem, we have at least one s.a. extension $\widetilde{\hat{f}} = \left(\widetilde{\hat{f}}\right)^+$ of the initial symmetric operator $\hat{f}$, given by $\widetilde{\hat{f}} = \hat{a}^+\overline{\hat{a}} + \hat{b} = \left(\overline{\hat{a}}\right)^+\overline{\hat{a}} + \hat{b} = \left(\widetilde{\hat{f}}\right)^+$, where $\overline{\hat{a}}$ is the closure of $\hat{a}$. This extension may be nonunique, but its existence guarantees that the deficiency indices of $\hat{f}$ are equal, and we can search for other s.a. extensions of $\hat{f}$ without fail.

2.9 Illustration by example of momentum operator

To illustrate the above-given general scheme, we consider a simplest one-dimensional quantum-mechanical system, a spinless particle moving on an interval (a, b) of a real axis $\mathbb{R}^1$, and a well-

known observable in this system, the momentum operator. The interval can be (semi)open or closed, the ends a and b can be infinities ($-\infty$ or $+\infty$). For the space of states of the system, we conventionally take the Hilbert space $L^2(a,b)$ whose vectors are wave functions $\psi(x)$, $x \in (a,b)$ (the x-representation). If we set the Planck constant $\hbar$ to be unity, $\hbar = 1$, then the standard well-known expression for the momentum operator is $\hat{p} = -id/dx$. But as we now realize, for the present, this formally s.a. "operator" is only a preliminary differential expression[24]

$$\check{p} = -i\frac{d}{dx} \tag{38}$$

because its domain is not prescribed in advance (by the known) quantization rules. The problem of quantization in this particular case is to construct a s.a. operator, an observable, associated with this differential expression. It turns out that the solution of this problem crucially depends on the type of the interval: whether it is a whole real axis, $(a,b) = (-\infty, +\infty) = \mathbb{R}^1$, or a semiaxis $(a,b) = [0,\infty)$ (a is taken to be zero for convenience, it can be any finite number) or $(a,b) = (-\infty, 0]$, or a finite segment[25] $[a,b]$, $-\infty < a < b < \infty$.

A most wide natural domain for a linear operator defined in $L^2(a,b)$ and given by the differential operation $-id/dx$ is the subspace D_* of wave functions $\psi_*(x) \in L^2(a,b)$ that are absolutely continuous on (a,b), the term "on" implies continuity up to the finite end or ends of the interval (a,b), and such that their derivative $\psi_*'(x)$ also belongs[26] to $L^2(a,b)$. We let $\hat{p}^*$ denote this operator, the above notation is justified below. The operator $\hat{p}^*$ is thus defined by[27]

$$\hat{p}^* : \left\{ \begin{array}{l} D_{p_*} = D_* = \{\psi_* : \psi_* \text{ a.c. on } (a,b) \,;\, \psi_*, \psi_*' \in L^2(a,b)\} \,, \\ \hat{p}^*\psi_* = \check{p}\psi_* = -i\psi_*' \,. \end{array} \right. \tag{39}$$

We first check the symmetricity of this operator (i.e., whether the equality $(\chi_*, \hat{p}^*\psi_*) - (\hat{p}^*\chi_*, \psi_*) = 0$ holds for any ψ_*, $\chi_* \in D_*$) and consider the difference

$$\omega_*(\chi_*, \psi_*) = (\chi_*, \hat{p}^*\psi_*) - (\hat{p}^*\chi_*, \psi_*) = -i\int_a^b dx \overline{\chi_*}\psi_*' - i\int_a^b dx \overline{\chi_*'}\psi_*, \ \forall \psi_*, \chi_* \in D_* \,. \tag{40}$$

A reader easily recognizes the sesquilinear asymmetry form of the operator $\hat{p}^*$ in ω_*. Integrating by parts in the second term, we find

$$\omega_*(\chi_*, \psi_*) = [\chi_*, \psi_*]|_a^b = [\chi_*, \psi_*](b) - [\chi_*, \psi_*](a) \,, \tag{41}$$

where we introduce a local sesquilinear form $[\chi_*, \psi_*]$ defined by

$$[\chi_*, \psi_*] = -i\overline{\chi_*(x)}\psi_*(x) \,, \tag{42}$$

and where $[\chi_*, \psi_*](a)$ and $[\chi_*, \psi_*](b)$ are the respective limits of this form as $x \to b, a$,

$$[\chi_*, \psi_*](a) = \lim_{x\to a}[\chi_*, \psi_*](x) \,, \ [\chi_*, \psi_*](b) = \lim_{x\to b}[\chi_*, \psi_*](x) \,. \tag{43}$$

[24]In what follows, we distinguish formal differential expressions from operators by an inverted hat $\vee$, see sec.3.

[25]Because the finite ends of an interval have a zero measure, we can include (or exclude) the finite ends in the interval. $L^2((a,b))$ and $L^2([a,b])$ are the same.

[26]Of course, we could extend D_* by step-functions that are also differentiable almost everywhere, but then there would be no possibility for integrating by parts and no chance for the symmetricity of the corresponding operator.

[27]In what follows, we use the abbreviation (a.c.=is absolutely continuous).

We call these limits the boundary values of the local form, or simply boundary term. These limits certainly exist because the integrals in r.h.s. of (40) do exist, they are the sesquilinear forms in the (asymptotic) boundary values of the wave functions in D_*. Eqs. (41,42) manifest that the sesquilinear asymmetry form of the differential operator $\hat{p}^*$ is reduced to the boundary values of the local form and the asymmetricity of $\hat{p}^*$ is defined by the asymptotic boundary values of the wave functions in D_* . At the moment, we have no ideas on the values of $[\chi_*, \psi_*](\pm\infty)$ in the case of infinite intervals. We must note that in the physical literature we can meet the assertion that the square-integrability of $\psi(x)$ at infinity, for example, $\psi \in L^2(-\infty, +\infty)$, $\int_{-\infty}^{+\infty} dx\, |\psi|^2 < \infty$, implies that ψ vanishes at infinity, $\psi(x) \to 0$ as $x \to \pm\infty$.

This is incorrect: it is a simple exercise to find a continuous function that is square-integrable at infinity but can take arbitrarily large values at arbitrarily large x. (To be true, in the following section we show that $[\chi_*, \psi_*](\pm\infty) = 0$ because ψ'_* is also square-integrable.)

On the other hand, what we certainly know is that in the case where one or both ends of an interval (a, b) are finite, for example, $|a| < \infty$ and/or $|b| < \infty$, we generally have $[\chi_*, \psi_*](a) = -i\overline{\chi_*}(a)\, \psi_*(a) \neq 0$ and/or $\overline{\chi_*}(b)\, \psi_*(b) \neq 0$, which implies that the operator $\hat{p}^*$ in this case is nonsymmetric.

There are two conclusions from this preliminary (perhaps excessively detailed and seemingly boring) consideration of this simple example, the conclusions that prove to be valid for more general differential expressions. First, a natural domain for a differential expression does not provide a symmetric operator in the case of finite boundaries. Second, the asymmetry form of a formally s.a. differential operator is defined by the boundary terms. It is a sesquilinear form in the (asymptotic) boundary values of functions involved (and their derivatives in the case of differential operators of higher order). Therefore, in order to guarantee the existence an initial symmetric operator associated with a given differential expression, it is necessary to take a more restricted domain of functions vanishing fast enough at the boundaries (and singularities) and yielding no contributions to the boundary terms.

In our case, we therefore restart with a domain $D(a, b)$ of finite smooth functions[28], $\overline{D(a, b)} = L^2(a, b)$, and respectively with a symmetric operator $\hat{p}^{(0)}$ defined by

$$\hat{p}^{(0)} : \begin{cases} D_{p^{(0)}} = D(a, b) = \{\varphi(x) : \varphi \in C^\infty,\ \operatorname{supp}\varphi \subset (a, b)\}, \\ \hat{p}^{(0)}\varphi = \check{p}\varphi = -i\varphi'. \end{cases} \tag{44}$$

The operator $\hat{p}^{(0)}$ is a restriction of the operator $\hat{p}^*$ to $D(a, b)$ and is evidently symmetric: the boundary terms $[\chi, \psi]|_a^b$ vanishes for any $\chi, \varphi \in D(a, b)$ because of the requirements on the support of functions in $D(a, b)$: they must vanish in a vicinity of the boundaries.

The first step of the general programme is thus completed.

We now must evaluate the adjoint $\left(\hat{p}^{(0)}\right)^+$. The defining equation for a pair $\psi_* \in D_{\left(p^{(0)}\right)^+}$ and $\chi_* = \left(\hat{p}^{(0)}\right)^+ \psi_*$,

$$\left(\psi_*, \hat{p}^{(0)}\varphi\right) - (\chi_*, \varphi) = 0\,,\ \forall \varphi \in D_{p^{(0)}} = D(a, b)\ ,$$

is

$$i\int_a^b dx \overline{\psi_*}\varphi' + \int_a^b dx \overline{\chi_*}\varphi = 0\,,\ \forall \varphi \in D(a, b)\ . \tag{45}$$

[28] This choice may seem too cautious in our case; however, $D(a, b)$ allows a universal consideration of symmetric operators with smooth coefficients of arbitrary order (see the following section).

We solve it using the following observation. We introduce an absolutely continuous function

$$\widetilde{\psi_*}(x) = i\int_c^x d\xi \chi_*(\xi) \ , \ a \le c \le b \tag{46}$$

such that $\chi_* = -i\widetilde{\psi_*}'$. Substituting (46) in (45) and integrating by parts in the second term, we reduce eq. (45) to

$$\int_a^b dx \left(\psi_* - \widetilde{\psi_*}\right)\varphi' = 0 \, , \ \forall\varphi \in D(a,b) \ .$$

(the boundary terms vanish because of $\varphi(x)$). By the known du Boi–Reymond lemma, it follows that $\psi_* - \widetilde{\psi_*} = c = \text{const}$, or

$$\psi_*(x) = i\int_c^x d\xi\chi_*(\xi) + c \, , \tag{47}$$

which implies that ψ_* is absolutely continuous on (a,b) and $\chi_* = \check{p}\psi_* = -i\psi_*'$. Conversely, any such function given by (47) evidently satisfies the defining equation (45).

This means that the adjoint $\left(\hat{p}^{(0)}\right)^+$ coincides with the above-introduced operator $\hat{p}^*$ given by (39), i.e., it is given by the same differential expression (38) and its domain is a natural one.

The second step of the general programme is also completed.

We now must evaluate the deficient subspaces and deficiency indices. It is this step where the difference in the type of the interval (a,b) manifests itself. The deficient subspaces $D_\pm$ are defined by the differential equations

$$-i\psi_\pm'(x) = \pm i\kappa\psi_\pm(x) \ , \ \psi_\pm \in D_* \subset L^2(a,b) \ ,$$

κ is an arbitrary, but fixed, parameter with the dimensionality of inverse length. The respective general solutions of differential equations (45) by itself are

$$\psi_\pm(x) = c_\pm e^{\mp\kappa x} \, , \tag{48}$$

where $c_\pm \in \mathbb{C}$ are constants.

Let $(a,b) = (-\infty,+\infty) = \mathbb{R}^1$, then both $\psi_\pm$ in (48) are non-square-integrable, ψ_+ is on $-\infty$ and ψ_- is on $+\infty$ unless $c_\pm \neq 0$. Therefore, in this case, the deficient subspaces are trivial, $D_\pm = \{0\}$, and the deficiency indices are zero, $m_+ = m_- = 0$, and the operator $\left(\hat{p}^{(0)}\right)^+ = \hat{p}^*$ (39) turns out to be symmetric (as we already mentioned above, the corresponding boundary terms are equal to zero). The operator $\hat{p}^{(0)}$ (44) is thus essentially s.a., and its unique s.a. extension is its closure, $\overline{\hat{p}^{(0)}} = \hat{p} = \left(\hat{p}^{(0)}\right)^+ = \hat{p}^*$; we let $\hat{p}$ denote the closure $\overline{\hat{p}^{(0)}}$.

The conclusion is that in the case $(a,b) = (-\infty,+\infty)$, there is only one s.a. operator associated with the differential expression $\check{p}$ (38). Passing to the physical language, we assert that for a spinless particle moving along the real axis $\mathbb{R}^1$, there is a unique momentum operator $\hat{p}$, an observable given by (we actually rewrite (39))

$$\hat{p} : \left\{ \begin{array}{l} D_p = \{\psi : \psi \text{ a.c. in } (-\infty,+\infty) \, ; \, \psi, \, \psi' \in L^2(\mathbb{R}^1)\} \ , \\ \hat{p}\psi = \check{p}\psi = -i\psi' \, . \end{array} \right. \tag{49}$$

A forth step is unnecessary. The spectrum, eigenfunctions and the physical interpretation of this operator are well-known.

Let $(a,b)=[0,\infty)=\mathbb{R}_{+}^{1}$, a semiaxis, then ψ_{+} in (48) is square-integrable, while ψ_{-} is not, unless $c_{-}=0$. We obtain that the deficiency indices of $\hat{p}^{(0)}$ in this case are $m_{+}=1$ and $m_{-}=0$ (in the case of $(a,b)=(-\infty,0]$, they interchange). This implies that in the case of a semiaxis, there is no s.a. operator associated with the differential expression $\check{p}$ (38). In the physical language, this means that for a particle moving on a semiaxis, the notion of momentum as a quantum-mechanical observable is absent. In particular, this implies the absence of the notion of radial momentum.

The general programme in the case of a semiaxis terminates at the third step.

Let now $(a,b)=[a,b]$, $0<a<b<\infty$, a finite segment, without loss of generality we take $[a,b]=[0,l]$, $l<\infty$. Then both ψ_{+} and ψ_{-} in (48) are square-integrable. This implies that in the case of a finite interval, the both deficient subspaces $D_{\pm}=\{c_{\pm}e_{\pm}(x)\}$, with $e_{+}=e^{-\kappa x}$ and $e_{-}=e^{-\kappa(l-x)}$ being the respective basis vectors of the same norm, are one-dimensional, such that the equal nonzero deficiency indices are $m_{+}=m_{-}=1$. According to the main theorem, this means that in the case of a finite interval, we have a one-parameter $U(1)$-family of s.a. operators associated with the differential expression $\check{p}$ (38) (the group $U(1)$ is a circle $\left\{e^{i\theta}\right\}$, $0\leq\theta\leq 2\pi$, $0\sim 2\pi$, the symbol $\backsim$ is the symbol of equivalence, or identification), and the fourth step is necessary.

We consider the both ways of specification given by the main theorem.

The first way requires evaluating the closure $\hat{p}=\overline{\hat{p}^{(0)}}$ of $\hat{p}^{(0)}$ (44), which reduces to finding its domain D_{p}. Equivalent defining equations for D_{p} are given in (13) and (15), or (16). We use the defining equation in (13), which in our case is $\omega_{*}\left(\psi_{*},\underline{\psi}\right)=0\,,\ \underline{\psi}\in D_{p}\,,\ \forall\psi_{*}\in D_{*}\,.$ According to (41), (42), this equation reduces to

$$i\left[\psi_{*},\underline{\psi}\right]\Big|_{0}^{l}=\overline{\psi_{*}(l)}\underline{\psi}(l)-\overline{\psi_{*}(0)}\underline{\psi}(0)=0\,,\ \forall\psi_{*}\in D_{*}\,,$$

a linear equation for the boundary values of functions in D_{p}. Because $\psi_{*}(0)$ and $\psi_{*}(l)$ can take arbitrary values independently, which, in particular, follows from representation (47), this yields $\underline{\psi}(0)=\underline{\psi}(l)=0\,.$

We obtain the same result considering the defining equation for D_{p} in (16), because the determinant of the boundary values of the basis vectors $e_{\pm}$ is nonzero,

$$\det\begin{pmatrix} e_{+}(l) & e_{+}(0)\\ e_{-}(l) & e_{-}(0)\end{pmatrix}=e^{-2\kappa l}-1\neq 0\,.$$

The closure $\hat{p}$ is thus specified by additional zero boundary conditions on the functions $\underline{\psi}$ in D_{p} in comparison with the functions ψ_{*} in D_{*} that can take arbitrary boundary values:

$$\hat{p}=\overline{\hat{p}^{(0)}}:\left\{\begin{array}{l} D_{p}=\left\{\underline{\psi}:\underline{\psi}\text{ a.c. on }[0,l];\,\underline{\psi},\underline{\psi}'\in L^{2}(0,l)\,,\,\underline{\psi}(0)=\underline{\psi}(l)=0\right\}\,,\\ \hat{p}\underline{\psi}=\check{p}\underline{\psi}=-i\underline{\psi}'\,.\end{array}\right. \tag{50}$$

The isometries $\hat{U}:D_{+}\rightarrow D_{-}$ are given by a complex number of unit module, $\hat{U}e_{+}=e^{i\theta}e_{-}\,,$ and are labelled by an angle θ, $0\leq\theta\leq 2\pi$, $0\backsim 2\pi$, $\hat{U}=\hat{U}(\theta)$. Respectively, the $U(1)$-family $\{\hat{p}_{\theta}\}$ of s.a. extensions of $\hat{p}^{(0)}$ (44), and $\hat{p}$ (50), is given by

$$\hat{p}_{\theta}:\left\{\begin{array}{l} D_{\theta}=D_{p_{\theta}}=\left\{\psi_{\theta}=\underline{\psi}+c\left(e^{-\kappa x}+e^{i\theta}e^{-\kappa(l-x)}\right)\right\}\,,\\ \hat{p}_{\theta}\psi_{\theta}=\check{p}\psi_{\theta}=-i\psi_{\theta}'\,,\end{array}\right. \tag{51}$$

where $\underline{\psi}$ is given by (50).

The second way of specification of s.a. extensions of $\hat{p}^{(0)}$, and $\hat{p}$, requires solving the defining equation for D_{p_θ} in (32), or (35). In our case, this equation, $\omega_*\left(e_+ + e^{i\theta}e_-, \psi_\theta\right) = 0$, reduces to

$$\left[e_+ + e^{i\theta}e_-, \psi_\theta\right]\Big|_0^l = -i\left(e^{-\kappa l} + e^{-i\theta}\right)\psi_\theta(l) + i\left(1 + e^{-i\theta}e^{-\kappa l}\right)\psi_\theta(0) = 0\,,$$

the equation relating the boundary values of functions in D_θ, and yields

$$\psi_\theta(l) = e^{i\vartheta}\psi_\theta(0)\ , \tag{52}$$

where the angle ϑ is

$$\vartheta = \theta - 2\arctan\left(\frac{\sin\theta}{e^{\kappa l} + \cos\theta}\right)\ . \tag{53}$$

The angle ϑ ranges from 0 to 2π when θ goes from 0 to 2π, $0 \leq \vartheta \leq 2\pi$, $0 \backsim 2\pi$, and is in one-to-one correspondence with the angle θ (it is sufficient to show that $\vartheta(\theta)$ is a monotonic function, $d\vartheta/d\theta > 0$); therefore, the angle ϑ equivalently labels the $U(1)$-family of s.a. extensions, which we write as $\hat{p}_\theta = \hat{p}_\vartheta$.

Eq. (52) is an additional boundary condition for the functions $\psi_\theta = \psi_\vartheta$ in $D_\theta = D_\vartheta$ in comparison with the functions $\psi_* \in D_*$. It is easy to verify that this boundary condition is equivalent to the representation ψ_θ in (51); therefore, this boundary condition is a s.a. boundary condition specifying the s.a. extensions as

$$\hat{p}_\vartheta : \left\{ \begin{array}{l} D_\vartheta = D_{p_\vartheta} = \left\{\psi_\vartheta : \psi_\vartheta \text{ a.c. on } [0,l]\ ;\ \psi_\vartheta, \psi'_\vartheta \in L^2(0,l);\ \psi_\vartheta(l) = e^{i\vartheta}\psi_\vartheta(0)\right\}\ , \\ \hat{p}_\vartheta\psi_\vartheta = \check{p}\psi_\vartheta = -i\psi'_\vartheta\,, \end{array} \right. \tag{54}$$

where $0 \leq \vartheta \leq 2\pi\,,\ 0 \backsim 2\pi\,$. The second specification seems more direct and explicit than the first one[29] because it specifies the s.a. extensions in the customary form of s.a. boundary conditions that are more suitable for spectral analysis.

The conclusion is that for a particle moving on a finite segment $[a,b]\,$, there is a one-parameter $U(1)$-family (a circle) of s.a. operators $\hat{p}_\vartheta = -id/dx$, that can be considered the momentum of a particle. These operators are labelled by an angle ϑ, and are specified by the s.a. boundary conditions $\psi_\vartheta(l) = e^{i\vartheta}\psi_\vartheta(0)$. In short, the momentum operator for a particle on a finite segment is defined nonuniquely.

The final step, the spectral analysis of these operators and the elucidation of their physical meaning, is postponed to a special publication.

We now turn to the general s.a. differential operators (in terms of which many observables in the quantum mechanics of particles are represented). We only note in advance that many key points of the above consideration of the momentum operator are characteristic for the general case.

3 Differential operators

3.1 Introduction

This section is devoted to differential operators, more specifically, to constructing s.a. differential operators associated with formal s.a. differential expressions[30]. We try to make it

[29] Although in the general form of the main theorem this appears to be the opposite.

[30] These notions are defined more precisely below.

as self-contained as possible and therefore don't afraid to repeat some items in the previous text. A reader who is acquainted with the end of the pervious section will see that some of the key points and remarks of the exposition to follow were already encountered in the above considerations.

We begin the section with remarks of the general character.

We restrict ourselves to ordinary differential operators in Hilbert spaces $L^2(a,b)$, $-\infty \leq a \leq b \leq \infty$ (scalar operators) with a special attention to examples from the nonrelativistic quantum mechanics of a one-dimensional motion (in particular, the radial motion) of spinless particles. But an extension to matrix differential operators in Hilbert spaces of vector-functions like $L^2(a,b) \oplus \ldots L^2(a,b)$ is direct. Therefore, the main results and conclusions of this section allow applying, with evident modifications, to the quantum mechanics of the radial motion of particles with spin, both nonrelativistic and relativistic, in particular, to the quantum mechanics of Dirac particles of spin 1/2.

As to partial differential operators, we refer to

[6, 17, 18, 19, 20, 21, 14, 3]; for physicists, we strongly recommend references [19] where three-dimensional Hamiltonians are classified and [3]. Foundations of the general theory of ordinary differential operators were laid by Weyl [22, 23, 24]. A somewhat different approach to the theory was developed by Titchmarsh [25, 17].

In view of many fundamental treatises on differential operators, our exposition is of a qualitative character in some aspects, a number of items is given under simplifying assumptions only to give basic ideas. But we try formulate the main statements and results for the general case as far as possible. By the mathematical tradition, we present them in the form of theorems. A physicist may find this manner superfluously mathematical, while a mathematician may find drawbacks in our formulations and proofs, but it provides a suitable system of references and facilitate applications.

All theorems are illustrated by simple, but we hope, instructive, examples of the well-known quantum mechanical operators like the momentum and Hamiltonian.

We additionally restrict ourselves to the case where possible singularities of the coefficient functions in a differential operator are on the boundaries (which is natural for radial Hamiltonians). If a singularity is located in the inner point c of an interval (a,b), like in the case of δ-potentials, the consideration must be appropriately modified. We here refer to the extensive treatise [28] on the subject.

And finally, the remarks directly related to our subject.

The general method of s.a. extensions of symmetric operators presented in the previous section and based on the main theorem is universal, i.e., it is universally applicable to symmetric operators of any nature. But as any universal method, it can turn out unsuitable as applied to some particular problems with their own specific features and therefore requires appropriate modifications. For example, in quantum mechanics for particles, nonrelativistic and relativistic, quantum-mechanical observables are usually defined in terms of s.a. differential operators, and the spectral problem is formulated as an eigenvalue problem for the corresponding differential equations[31]. In the presence of boundaries and/or singularities of the potential, we are used to accompany these equations with one or another boundary conditions on the wave functions. This means that we additionally specify the domain of the corresponding observables by the

[31]Of course, this does not concern the spin degrees of freedom and spin systems where observables are represented by Hermitian matrices.

boundary conditions that provide the self-adjointness of the differential operators under consideration. It is natural to call such boundary conditions the s.a. boundary conditions, this is a standard term in the mathematical literature.

A revealing of the specific features of s.a. extensions of differential symmetric operators is just the subject if this section.

It appears that in the case of differential operators, the isometries $\hat{U} : D_+ \to D_-$ of one deficient subspace to another specifying s.a. extensions of symmetric operators can be converted into s.a. boundary conditions, explicit or implicit. This possibility is based on the fact that the asymmetry forms ω_* and Δ_* are expressed in terms of asymptotic boundary values of functions and their derivatives. In addition to conventional methods, we discuss a possible alternative way of specifying s.a. differential operators in terms of explicit boundary conditions. It is based on direct modification of the arguments resulting in the main theorem. The method does not require evaluating the deficient subspaces D_+ and D_- and the deficiency indices, the latter are determined in passing. Its effectiveness is illustrated by a number of examples of quantum-mechanical operators. Unfortunately, this method is not universal at present. Its applicability depends on to what extent we can establish the boundary behavior of functions involved. In general, it depends on specific features of boundaries, in particular, whether they are regular or singular.[32]

3.2 Differential expressions

Let (a,b) be an interval of the real axis $\mathbb{R}^1$. By (a,b) we mean an interval in a generalized sense: the ends a and b of the interval can be infinite, $a=-\infty$ and/or $b=+\infty$; if they are finite, $|a|<\infty$ and/or $|b|<\infty$, they can be included in the interval such that we can have a pure interval (a,b), semi-interval $[a,b)$ or $(a,b]$, or a segment $[a,b]$. This depends on the regularity of the coefficients of a differential operator under consideration.

Each interval (a,b) is assigned the Hilbert space $L^2(a,b)$ of functions, wave functions in the physical terminology. We recall that from the standpoint of Hilbert spaces, the inclusion of the finite end points a and/or b in (a,b) is irrelevant: the Hilbert spaces $L^2((a,b))$ and $L^2([a,b])$ for the respective pure interval (a,b) and segment $[a,b]$ are the same because the Lebesgue measure of a point is zero.

A differential expression, or a differential operation, $\check{f}$ associated with an interval (a,b) is an expression of the form

$$\check{f} = f_n(x)\left(\frac{d}{dx}\right)^n + f_{n-1}(x)\left(\frac{d}{dx}\right)^{n-1} + \cdots + f_1(x)\frac{d}{dx} + f_0(x) \ , \ x \in (a,b) \ , \qquad (55)$$

where $f_k(x)$, $k=0,1,\ldots,n$, are some functions on (a,b) that are called the coefficient functions, or simply coefficients, of the differential expression, $f_n(x)\neq 0$; an integer $n\geq 1$ is called the order of $\check{f}$.

The differential expression $\check{f}$ naturally defines a linear differential operator over functions on (a,b), whence an alternative name "differential operation" for $\check{f}$,

$$\left(\check{f}\psi\right)(x) = f_n(x)\psi^{(n)}(x) + f_{n-1}(x)\psi^{(n-1)}(x) + \cdots + f_1(x)\psi'(x) + f_0(x)\psi(x) \ , \qquad (56)$$

[32]These notions are explained below.

under the natural assumption that ψ is absolutely continuous together with its $n-1$ derivatives[33] $\psi^{(1)} = \psi', \ldots, \psi^{(n-1)}$. Formula (56) defines the "rule of acting" for future operators in $L^2(a,b)$.

An intermediate remark is in order here.

The consideration to follow are directly extended to matrix deferential expressions, i.e., to deferential expressions with matrix coefficients, that generate systems of differential equations and differential operators in Hilbert space of vector-functions like $L^2(a,b) \oplus \cdots \oplus L^2(a,b)$ where vector-functions are columns of square-integrable functions. Such matrix differential expressions are inherent in nonrelativistic and relativistic quantum mechanics of particles with spin, in particular, Dirac particles (we mean the radial motion of particles).

As is well known, an ordinary differential equation of order n can be reduced to a system of n first-order differential equations, and vice versa. What is more, this reduction is useful in analyzing homogeneous an inhomogenous differential equations, in particular, in establishing the structure of their general solution. Respectively, any differential expression $\check{f}$ (55) is assigned a first-order matrix differential expression with $n \times n$ matrix coefficients.

The regularity conditions for the coefficients f_k (integrability, continuity, differentiability, etc.) depend on the context. The standard conditions are that f_k, $k = 1, \ldots, n-1$, has k derivatives in (a,b), $f_n \neq 0$, and f_0 is locally integrable[34] in (a,b); the coefficients, for example, f_0, can be infinite as $x \to a$ and/or $x \to b$. These conditions are sufficient for the function $\check{f}\psi$ to allow integrating by parts and a given differential expression $\check{f}$ to have an adjoint differential expression $\check{f}^*$, see below, and for the functions $f_0, f_1, \ldots, f_{n-1}$ and $1/f_n$ to be locally integrable in (a,b), which is necessary for the theory of usual differential equations generated by a given differential expression: the homogenous equation $\check{f}\psi = 0$ and the inhomogenous equation $\check{f}\psi = \chi$, see below. The conditions on the coefficients sometimes can be considerably weakened for another representation of differential expressions, see below. For the first reading, one can consider the coefficients f_k smooth functions. If the coefficients have singularities in (a,b), a separate special consideration is required.

In the physical language, $\check{f}$ (55) can be considered an element of a formal algebra generated by the "operators" $\hat{q} = x$ (the position operator) and $\hat{p} = -id/dx$ (the momentum operator[35]), satisfying the canonical commutation relation $[\hat{q}, \hat{p}] = i$,

$$\check{f} = f_n(\hat{q})(i\hat{p})^n + f_{n-1}(\hat{q})(i\hat{p})^{n-1} + \cdots + f_1(\hat{q})\, i\hat{p} + f_0(\hat{q}) \ ,$$

with the so-called *qp*-ordering [3].

The differential expression (55) is called the regular differential expression if the interval (a,b) is finite and if the coefficients $f_0, \ldots, f_{n-1}$, and the function f_n^{-1} are integrable[36] on (a,b), the term "on (a,b)" means on the whole (a,b), including the ends a and b; in this case, we consider (a,b) as a segment $[a,b]$. In the opposite case, $\check{f}$ is called the singular differential expression. The left end a is called the regular end if $a > -\infty$, and the indicated functions

[33] $\psi^{(k)}$ is a conventional symbol of the derivative of order k.

[34] It is integrable on any finite interval inside (a,b).

[35] The Planck constant $\hbar$ is set to unity, $\hbar = 1$. In the mathematical language, $\hat{q}$ and $\hat{p}$ are called the generators of the algebra, or "symbols". We no longer use the physical symbol $f(\hat{q}, \hat{p}) = f\left(x, -i\frac{d}{dx}\right)$, or more briefly $f\left(x, \frac{d}{dx}\right)$, for $\check{f}$, because its origin is irrelevant here.

[36] This condition does not exclude that the coefficients, for example, $f_0(x)$, can be infinite as $x \to a$ and/or $x \to b$.

are integrable on any segment $[a,\beta]$, $\beta<b$. In the opposite case, i.e., if $a=-\infty$ and/or the integrability condition on $[a,\beta]$ for the coefficients does not hold, the end a is called the singular end. Similar notions are introduced for the right end.

Let $\varphi(x)$ and $\phi(x)$ be smooth finite functions, $\varphi,\phi\in D(a,b)$, then the function $\check{f}\varphi$ is square-integrable[37] on (a,b), as well as φ, and the scalar product $(\phi,f\varphi)=\int_a^b dx\overline{\phi}\check{f}\varphi$ has a sense. We consider this integral. Integrating by parts and taking into account that the standard boundary terms vanish because of finite supports of φ and ϕ, we have

$$(\phi,\check{f}\varphi)=\int_a^b dx\overline{\phi}\check{f}\varphi=\int_a^b dx\overline{\check{f}^*\phi}\varphi=\left(\check{f}^*\phi,\varphi\right)\,, \tag{57}$$

where the function $\check{f}^*\varphi$ is given by

$$\check{f}^*\phi=\left(-\frac{d}{dx}\right)^n(\overline{f_n}\phi)+\left(-\frac{d}{dx}\right)^{n-1}(\overline{f_{n-1}}\phi)+\cdots+\left(-\frac{d}{dx}\right)(\overline{f_1}\phi)+\overline{f_0}\phi\,, \tag{58}$$

and defines the differential expression

$$\check{f}^*=\left(-\frac{d}{dx}\right)^n\overline{f_n}+\left(-\frac{d}{dx}\right)^{n-1}\overline{f_{n-1}}+\cdots+\left(-\frac{d}{dx}\right)\overline{f_1}+\overline{f_0}\,, \tag{59}$$

a differential operation each term $\left(-\frac{d}{dx}\right)^k\overline{f_k}$ of which implies first multiplying a function by the function $\overline{f_k}$ and then differentiating the result k times, which has a sense on the above-given set of functions because $f_k(x)$ is k-time-differentiable. The differential expression $\check{f}^*$ (59) is called the the adjoint differential expression (to $\check{f}$), or simply the adjoint, or the adjoint by Lagrange. In the physical language, the adjoint is defined by

$$\check{f}^*=(-i\hat{p})^n\,\overline{f_n}(\hat{q})+(-i\hat{p})^{n-1}\,\overline{f_{n-1}}(\hat{q})+\cdots-i\hat{p}\overline{f_1}(\hat{q})+\overline{f_0}(\hat{q})\,, \tag{60}$$

it is the adjoint in the above-mentioned formal algebra with involution (the standard rule for taking the adjoint: reversing the order of "operators" and the complex conjugation of the numerical coefficients, which is denoted by a bar over the function symbol. It naturally arises as a pq-ordered expression. The adjoint $\check{f}^*$ (59) can be reduced to form (55),

$$\begin{aligned}\check{f}^*=\overline{f_n}\left(-\frac{d}{dx}\right)^n&+\left[\overline{f_{n-1}}-n\overline{f_n'}\right]\left(-\frac{d}{dx}\right)^{n-1}+\cdots+\left[\overline{f_1}+\cdots+(-1)^{n-2}(n-1)\,\overline{f_{n-1}^{(n-2)}}\right.\\&\left.+(-1)^{n-1}\,n\overline{f_n^{(n-1)}}\right]\left(-\frac{d}{dx}\right)+\left[\overline{f_0}+\cdots+(-1)^{n-1}\,\overline{f_{n-1}^{(n-1)}}+(-1)^n\,\overline{f_n^{(n)}}\right]\,,\end{aligned} \tag{61}$$

by subsequently differentiating in r.h.s. of (58) and using the Leibnitz rule, or by rearranging the pq-ordering in (60) to the qp-ordering by subsequently commuting all $\hat{p}$'s in $\hat{p}^k=\hat{p}\cdots\hat{p}$ with $f_k(\hat{q})$ with the rule

$$\hat{p}\overline{f_k^{(l)}}(\hat{q})=\overline{f_k^{(l)}}(\hat{q})\,\hat{p}+\left[\hat{p},\overline{f_k^{(l)}}(\hat{q})\right]=\overline{f_k^{(l)}}(\hat{q})\,\hat{p}+(-i)\,\overline{f_k^{(l+1)}}(\hat{q})\,,\;l=0,1,\ldots,k-1\,.$$

A reader can easily write a detailed formula.

[37] Because of our conditions for the coefficients of $\check{f}$ and because of a finite support of φ and therefore of $\check{f}\varphi$.

A differential expression $\check{f}$ is called a s.a. differential expression, or s.a. by Lagrange , if it coincides with its adjoint, $\check{f} = \check{f}^{*}$.

Any differential expression $\check{f}$ can be assigned a differential operator in $L^{2}(a,b)$ if an appropriate domain in $L^{2}(a,b)$ for this operator with the "rule of acting" given by $\check{f}$ is indicated. But only a s.a. differential expression can generate a s.a. differential operator in $L^{2}(a,b)$, which is of interest from the standpoint of quantum mechanics. We refer to such an operator as a s.a. operator associated with a given s.a. differential expression. The self-adjointness of a differential expression is only necessary for the existence of the respective s.a. operator and in general is not sufficient: the main problem is to indicate the proper domain in $L^{2}(a,b)$ such that $\check{f}$ becomes a s.a. operator, sometimes, it appears impossible; in addition, different s.a. operators can be associated with the same differential expression as we already know from the example at the end of the previous section.

We now describe the general structure of s.a. differential expressions of any finite order that makes its self-adjointness obvious.

The coefficients of a s.a. differential expression $\check{f}$ (55), $\check{f} = \check{f}^{*}$, satisfy the following conditions with respect to complex conjugation:

$$
\begin{aligned}
&\overline{f_n} = (-)^{n} f_n \,, \\
&\overline{f_{n-1}} = (-)^{n-1} f_n + (-)^{n} n f_n^{(1)} \,, \\
&\vdots \\
&\overline{f_1} = -f_1 + \cdots + (-)^{n-1}(n-1) f_{n-1}^{(n-2)} + (-)^{n} n f_n^{(n-1)} \,, \\
&\overline{f_0} = f_0 + \cdots + (-)^{n-1} f_{n-1}^{(n-1)} + (-)^{n} f_n^{(n)} \,,
\end{aligned}
$$

that follow from the comparison of r.h.s. in (55) with r.h.s. in (61) and the subsequent complex conjugation. These conditions can be resolved, which leads to the so-called canonical form of a s.a. differential expression. The canonical form of a s.a. differential expression is a sum of s.a. odd binomials,

$$
\begin{aligned}
\check{f}_{(2k-1)} &= \frac{i}{2}\left[\left(\frac{d}{dx}\right)^{k-1} f_{2k-1}\left(-\frac{d}{dx}\right)^{k} + \left(-\frac{d}{dx}\right)^{k} f_{2k-1}\left(\frac{d}{dx}\right)^{k-1}\right] , \\
f_{2k-1} &= \overline{f_{2k-1}},\ k = 1,2,\ldots,
\end{aligned}
\tag{62}
$$

and s.a. even monomials,

$$
\check{f}_{(2k)} = \left(-\frac{d}{dx}\right)^{k} f_{2k}\left(\frac{d}{dx}\right)^{k} ,\ f_{2k} = \overline{f_{2k}}\,,\ k = 0,1,\ldots\ , \tag{63}
$$

with the real coefficient functions f_l ($f_{(0)} = f_0(x)$ is here considered a differential expression of order zero); for brevity, we use the same notation for the coefficient functions as for those in (55).

In terms of the formal algebra, these are the respective "operators"

$$
\check{f}_{(2k-1)} = \frac{1}{2}\left[\hat{p}^{k-1} f_{2k-1}(\hat{q})\, \hat{p}^{k} + \hat{p}^{k} f_{2k-1}(\hat{q})\, \hat{p}^{k-1}\right] ,\ k = 1, 2\,, \ldots,
$$

and

$$\check{f}_{(2k)} = \hat{p}^k f_{2k}(\hat{q})\,\hat{p}^k\,,\ k = 0, 1, \dots\,,$$

with the properly symmetrized pq-ordering; they are well-known to physicists [3].

The canonical form of a s.a. differential expression $\check{f} = \check{f}^*$ of order $n \geq 1$ is thus given by

$$\check{f} = \sum_k \check{f}_{(2k)} + \sum_k \check{f}_{(2k+1)} \tag{64}$$

In this form (64) for a s.a. differential expression, the regularity conditions for the coefficient functions $f_l(x)$ can be weakened: there is no need in the l-time-differentiability of $f_l(x)$, a natural sufficient requirement is that $f_{2k}(x)$ and $f_{2k-1}(x)$ be only k-time-differentiable.

The simplest first-order s.a. differential expression is $\check{f} = \check{p}$ given by (38) that is identified in physics with the quantum mechanical momentum of a particle moving on an interval (a, b) of a real axis; it was considered at the end of the previous section.

The even second-order differential expression with the conventional notation $f_2(x) = p(x)$, $f_0(x) = q(x)$ is the Sturm-Lioville differential expression

$$\check{f} = -\frac{d}{dx}p(x)\frac{d}{dx} + q(x)\ ,\ p(x) = \overline{p(x)}\,,\ q(x) = \overline{q(x)}\,.$$

With $p(x) = 1$ and $q(x) = V(x)$, we let $\check{H}$ denote $\check{f}$ and obtain the second-order s.a. differential expression

$$\check{H} = -\frac{d^2}{dx^2} + V(x) \tag{65}$$

that is identified in physics with the quantum-mechanical Hamiltonian[38] for a nonrelativistic particle moving on an interval (a, b) of the real axis in the potential field $V(x)$. In what follows, we mainly deal with this simplest, but physically interesting, differential expression (65) when illustrating the general assertions.

The general even s.a. differential expression of order n,

$$\check{f} = \sum_{k=0}^{n/2}\left(-\frac{d}{dx}\right)^k f_{2k}\left(\frac{d}{dx}\right)^k\,,\ f_{2k} = \overline{f_{2k}}\,, \tag{66}$$

can be rewritten in terms of differential operations $D^{[k]}$, $k = 1, \dots, n$, that are defined recursively and separately for each $\check{f}$ by

$$D^{[k]} = \left(\frac{d}{dx}\right)^k\,,\ k = 1, \dots, n/2 - 1\,,\ D^{[n/2]} = f_n\left(\frac{d}{dx}\right)^{n/2}\,,$$

$$D^{[n/2+k]} = f_{n-2k}\left(\frac{d}{dx}\right)^{n-2k} - \frac{d}{dx}D^{[n/2+k-1]}\,,\ k = 1, \dots, n/2\,,$$

and define the respective so-called quasi-derivatives [7, 8] by[39]

$$\psi^{[k]} = D^{[k]}\psi \Longrightarrow \begin{cases} \psi^{[k]} = \psi^{(k)}\,,\ k = 1, \dots, n/2 - 1\,,\ \psi^{[n/2]} = f_n\psi^{(n/2)}\,, \\ \psi^{[n/2+k]} = f_{n-2k}\psi^{(n-2k)} - \frac{d}{dx}\psi^{[n/2+k-1]}\,,\ k = 1, \dots, n/2\,. \end{cases}$$

[38] To be true, this identification assumes appropriate units, where, for example, the Planck constant $\hbar = 1$ and the mass of a particle $m = 1/2$; with the usual units, differential expression (65) corresponds to the Hamiltonian multiplied by a numerical factor $\frac{2m}{\hbar^2}$.

[39] In [7, 8], an even n is denoted by $2n$, and the coefficient functions $f_{2k}(x)$ are denoted by $p_{n-k}(x)$: $p_{n-k}(x) = f_{2k}(x)$.

Then the differential expression (66) is simply written as

$$\check{f} = D^{[n]}\,, \tag{67}$$

and

$$\check{f}\psi = \psi^{[n]}\,. \tag{68}$$

With this form (67) for $\check{f}$ (66) and (68) for $\check{f}\psi$, the regularity conditions for the coefficient functions f_{2k} can be essentially weakened: it is not necessary that f_{2k} be k-time differentiable; it is sufficient that $\psi^{[k]}$, $k = 1, \ldots, n-1$, be absolutely continuous in (a, b) for $\psi^{[n]}$ to have a sense and that the functions $f_0, \ldots, f_{n-2}, 1/f_n \neq 0$ be locally integrable for the homogenous and inhomogenous differential equations $\check{f}\psi = 0$ and $\check{f}\psi = \chi$ to be solvable with usual properties of their general solution. The notions of regular and singular ends are modified respectively.

Any even s.a. expression $\check{f}$ (66), (67) is assigned at least one associated s.a. operator (see below). The notion of quasi-derivatives allows highly elaborating the theory of even s.a. differential operators with real coefficients [7, 8]. To our knowledge, there is no similar notion for odd s.a. differential expressions and for the respective s.a. differential operators with imaginary coefficients. For any s.a. differential expression (64) of any order n, the so called Lagrange identity

$$\overline{\chi}\check{f}\psi - \left(\overline{\check{f}\chi}\right)\psi = \frac{d}{dx}\left[\chi, \psi\right] \tag{69}$$

holds, where $[\chi, \psi]$ is a local sesquilinear form in functions and their derivatives of order up to $n-1$:

$$\begin{aligned}
\left[\chi, \psi\right] &= -i\sum_{k=1}^{\left[\frac{n+1}{2}\right]}\overline{\chi^{(k-1)}}f_{2k-1}\psi^{(k-1)} + \frac{i}{2}\sum_{k=2}^{\left[\frac{n+1}{2}\right]}\sum_{l=0}^{k-2}\left\{\overline{\chi^{(l)}}\left(-\frac{d}{dx}\right)^{k-2-l}\right. \\
&\times\left[\left(f_{2k-1}\psi^{(k)}\right) + \left(f_{2k-1}\psi^{(k-1)}\right)'\right] + \left(-\frac{d}{dx}\right)^{k-2-l}\left.\left[\left(f_{2k-1}\overline{\chi^{(k)}}\right) + \left(f_{2k-1}\overline{\chi^{(k-1)}}\right)'\right]\psi^{(l)}\right\} \\
&+\sum_{k=1}^{\left[\frac{n}{2}\right]}\sum_{l=0}^{k-1}\left[\psi^{(k)}\left(-\frac{d}{dx}\right)^{k-l-1}\left(f_{2k}\overline{\chi^{(k)}}\right) - \overline{\chi^{(l)}}\left(-\frac{d}{dx}\right)^{k-l-1}\left(f_{2k}\psi^{(k)}\right)\right]\,.
\end{aligned} \tag{70}$$

Equalities (69), (70) can be derived by the standard procedure of subsequently extracting a total derivative in the l.h.s. of (69) used in integrating by parts or can be verified directly by differentiating $[\chi, \psi]$ (70) in the r.h.s. of (69).

It follows the integral Lagrange identity

$$\int_\alpha^\beta dx\overline{\chi}\check{f}\psi - \int_\alpha^\beta dx\psi\overline{\check{f}\chi} = \left[\chi, \psi\right]\big|_\alpha^\beta\,, \tag{71}$$

where $[\alpha, \beta]$ is any finite segment of (a, b), $[\alpha, \beta] \subset (a, b)$, and, by definition, $[\chi, \psi]|_\alpha^\beta$ is the difference of the form $[\chi, \psi]$ at the respective points β and α:

$$\left[\chi, \psi\right]\big|_\alpha^\beta = \left[\chi, \psi\right](\beta) - \left[\chi, \psi\right](\alpha).$$

As simple examples, for first-order differential expressions (38), we have $\left[\chi, \psi\right](x) = -i\overline{\chi(x)}\psi(x)$, while for the second-order deferential expression (65), we have

$$\left[\chi, \psi\right](x) = -\left[\overline{\chi(x)}\psi'(x) - \overline{\chi'(x)}\psi(x)\right]\,. \tag{72}$$

We point out some properties of the form $[\chi, \psi]$. We first note that the conventional symbol $[\cdot, \cdot]$ for this form is identical to the symbol of a commutator (perhaps, this is because the l.h.s. of (69) is similar to a commutator and because in the framework of the commutative algebra of functions there is no need in the symbol of a true commutator, so that a confusion is avoided). But $[\chi, \psi]$ is not a commutator, and, in particular, $[\psi, \psi] \neq 0$ in general.

For even s.a. expressions $\check{f}$ (66), (67) of order n, the form $[\chi, \psi]$ is a simple sesquilinear form in quasi-derivatives:

$$[\chi, \psi] = -\sum_{k=0}^{n/2-1} \left(\overline{\chi^{[k]}} \psi^{[n-k-1]} - \overline{\chi^{[n-k-1]}} \psi^{[k]} \right) . \tag{73}$$

We note that because the coefficient functions of even s.a. expressions are real, we have $[\overline{\psi}, \psi] \equiv 0$, $\forall \psi$, while $[\psi, \psi] \neq 0$ in general unless ψ is real up to a constant factor of module unity, $\overline{\psi} = e^{i\theta}\psi$, $\theta = \text{const}$.

The form $[\chi, \psi]$ (70) is evidently antisymmetric, $\overline{[\chi, \psi]} = -\underline{[\psi, \chi]}$, and its reduction to the diagonal $\chi = \psi$, the quadratic form $[\psi, \psi]$, is purely imaginary, $\overline{[\psi, \psi]} = -[\psi, \psi]$. Let the functions ψ and χ in $[\chi, \psi]$ satisfy the same homogenous linear differential equation generated by a s.a. expression $\check{f}$, $\check{f}\psi = 0$ and $\check{f}\chi = 0$; we note that if $\check{f}$ is odd with pure imaginary coefficients or even with real coefficients, the complex conjugate functions $\overline{\psi}$ and $\overline{\chi}$ satisfy the same equation. It simply follows from (69) that the form $[\chi, \psi]$ (70) for solutions of the homogenous equation does not depend on x, i.e., $[\chi, \psi] = \text{const}$. For second-order differential expressions this is a well-known fact: a reader can easily recognize the Wronskian for $\overline{\chi}$ and ψ in (72). We only note that this is the Wronskian for $\overline{\chi}$, which is also a solution of the homogenous equation, and ψ, but not for χ and ψ in particular, $[\psi, \psi]$ which is the Wronskian for $\overline{\psi}$ and ψ, is generally not equal to zero; this is a specific feature of the complex linear space under consideration.

The same is true if ψ and χ are the solutions of the respective spectral equations $\check{f}\psi = \lambda\psi$ and $\check{f}\chi = \overline{\lambda}\chi$ with complex conjugated parameters. We again note that if $\check{f}\psi = \lambda\psi$ then for an odd s.a. differential expressions, we have $\check{f}\overline{\psi} = -\overline{\lambda\psi}$, while for an even s.a. differential expressions, we have $\check{f}\overline{\psi} = \overline{\lambda\psi}$.

3.3 Differential equations

Before we turn to differential operators generated by s.a. differential expression, we must recall some facts of the theory of ordinary differential equations, homogenous and inhomogenous.

The theory of s.a. differential operators in $L^2(a, b)$ is based on the theory of ordinary linear differential equations, especially on the theory of its general solutions including the so-called generalized ones. We recall the basic points of this theory as applied to homogenous and inhomogenous differential equations generated by the above-introduced s.a. differential expressions. We present them by the simple examples of differential expressions (38) of the first order and (65) of the second order. On the one hand, these expressions are of physical interest and are widely used in physical applications, on the other hand, they allow demonstrating the common key points of the general consideration.

As to the simplest first-order differential expression (38), this programme has been accomplished above, in the end of the previous section. The general solutions of the corresponding equation $-i\frac{d}{dx}y(x) = 0$ and $-i\frac{d}{dx}y(x) = h(x)$ are so obvious that this allows completely

solving all the problems related to this differential expression, including s.a. operators. The consideration was so easy that some general points could prove to be somewhat hidden.

We therefore proceed to differential expression (65). This differential expression is correctly defined as a differential operator on the complex linear space of functions on (a, b) that are absolutely continuous in (a, b) together with their first derivatives. We change the notation of functions from $\psi(x), \chi(x), \ldots$, which is usually adopted in physics for functions in $L^2(a, b)$, to $u(x), y(x), \ldots$, which is usually adopted in the theory of differential equations, in particular, because these functions are generally non-square-integrable on an arbitrary interval $(a, b) \subseteq \mathbb{R}^1$.

On this space, we consider the homogenous differential equation

$$\check{H}u = -u'' + Vu = 0 \tag{74}$$

and the inhomogenous differential equation

$$\check{H}y = -y'' + Vy = h\,, \tag{75}$$

where $h(x)$ is assumed to be locally integrable.

It is known from the theory of ordinary differential equations that if V is locally integrable, eq. (74) has two linearly independent solutions u_1 and u_2, $\check{H}u_{1,2} = 0$, that form a fundamental system of eq. (74) in the sense that the general solution of eq. (74) is

$$u = c_1 u_1 + c_2 u_2\,, \tag{76}$$

where c_1 and c_2 are arbitrary complex constants, these constants are fixed by initial conditions on u and u' at some inner point in (a, b) or at a regular end. The linear independence of u_1 and u_2 is equivalent to the requirement that their Wronskian $W(u_1, u_2) = u_1(x)\, u_2'(x) - u_2(x)\, u_1'(x)$, which is a constant for any two solutions of eq. (74), be nonzero, $W(u_1, u_2) = \text{const} \neq 0$. Of course, the fundamental system u_1, u_2 is defined up to a nonsingular linear transformation. For real potentials, $V = \overline{V}$, the functions u_1 and u_2 can also be taken to be real . If the end a of the interval (a, b) is regular, i.e., if $-\infty < a$ and V is integrable up to a, i.e., $\int_a^\beta dx\,|V| < \infty$, $\beta < b$, then any solution (76) has a finite limit at this end together with its first derivative. The same is true for a regular right end b. In the case of singular ends, one or both of fundamental solutions, i.e., u_1, u_1' and/or u_2, u_2', can be infinite at such ends. If the potential V is smooth in (a, b), $V \in C^\infty(a, b)$, which does not exclude that V is infinite at the ends, then any solution u (76) is also smooth in (a, b).

The general solution of inhomogenous equation (75) is given by

$$y(x) = \frac{1}{W(u_1, u_2)} \left[u_1(x) \int_\alpha^x d\xi\, u_2 h + u_2(x) \int_x^\beta d\xi\, u_1 h \right] + c_1 u_1(x) + c_2 u_2(x)\,,$$

where α and β are arbitrary, but fixed, inner points in (a, b), in particular, we can choose $\alpha = \beta$, and c_1 and c_2 are arbitrary constants that are fixed by initial conditions on y and y' at some inner point in (a, b) or at a regular end. If the left end a of the interval (a, b) is regular, we can always take $\alpha = a$, we can also do this in the case where the end a is singular if the respective integral is certainly convergent, for example, if the functions u_2 and h are square-integrable on the segment $[a, x]$; the same is true for the right end b.

We now consider the question about the so-called generalized solutions of homogenous equation (74), i.e., the question about functions u that satisfy the linear functional equation

$$\int_a^b dx\, \overline{u}\check{H}\varphi = 0\,,\ \forall\varphi \in D(a, b)\ . \tag{77}$$

Generally speaking, u in (77) can be considered a generalized function (a distribution), then the integral in (77) is symbolical, but for our purposes, it appears sufficient that u be a function[40]. It is evident that any usual solution (76) of homogenous equation (74) is a generalized solution, i.e., satisfies eq. (77) because of the equality

$$\int_a^b dx \overline{y} \check{H} \varphi = \int_a^b dx \varphi \overline{\check{H} y}\,,\ \forall \varphi \in D(a,b)\ , \tag{78}$$

for any function y absolutely continuous in (a,b) together with its derivative y', which follows from integrating by parts in l.h.s. in (78) with vanishing boundary terms because of a finite support of φ, $\operatorname{supp}\varphi \subseteq [\alpha,\beta] \subset (a,b)$, i.e., because φ vanishes in a neighborhood of the limits of integration. Actually, eq. (78) is a particular case of the extension of eq. (57) for s.a. differential expressions $\check{f} = \check{f}^*$ of any order n from functions $\phi \in D(a,b)$ to functions y absolutely continuous in (a,b) together with its $n-1$ derivatives,

$$\int_a^b dx \overline{y} \check{f} \varphi = \int_a^b dx \varphi \overline{\check{f} y}\,, \tag{79}$$

for the validity of equality (79), it is sufficient that only $\varphi \in D(a,b)$. We would like to show that conversely, any generalized solution of homogenous equation is a usual solution, i.e., any solution $u(x)$ of eq. (77) is given by eq. (76).

Here, we make a simplifying technical assumption that the potential V is a smooth function, $V \in C^\infty(a,b)$, and $\check{H}\varphi \in D(a,b)$ as well as φ, which allows making use of the well-developed theory of distributions (strictly speaking, $u(x)$ in (77) can be considered a distribution only in this case).

This assumption is in fact technical; the main result can be extended to the general case, see below. We also note that many potentials encountered in physics satisfy this condition. But if V is nonsmooth, no practical loss of generality from the standpoint of constructing s.a. operators associated with $\check{H}$ occurs. Let the potential V be a locally bounded function, i.e., it is bounded in any finite segment $[\alpha,\beta] \subset (a,b)$, with possible finite jumps, such that step-like potentials or barriers are admissible. Any such potential can be smoothed out, i.e., approximated by a smooth potential $V_{\text{reg}}(x)$, such that the difference $\delta V = V(x) - V_{\text{reg}}(x)$ is uniformly bounded. Then the operators $\hat{H}$ and $\hat{H}_{\text{reg}}$ in $L^2(a,b)$ associated with the respective differential expressions (65) and $\check{H}_{\text{reg}} = -\frac{d^2}{dx^2} + V_{\text{reg}}(x)$ differ by a bounded s.a. multiplication operator $\widehat{\delta V} = \delta V(x)$ defined everywhere, $\hat{H} - \hat{H}_{\text{reg}} = \widehat{\delta V}$, and, therefore, are s.a. or non-s.a. simultaneously, more precisely, any s.a. operator $\hat{H}_{\text{reg}}$ is assigned a s.a. operator $\hat{H} = \hat{H}_{\text{reg}} + \widehat{\delta V}$ with the same domain, and vice-versa.

Let thus the potential V be smooth, and we return to the problem of the generalized solutions of homogenous equation (74), i.e., the solutions of eq. (77). We actually need a generalization of the du Boi–Reymond lemma used at the end of the previous section when constructing s.a. operators associated with the first-order differential expression $\check{p}$ (38). We obtain this generalization based on two auxiliary lemmas. In the process, it becomes clear how the result on the generalized solutions can be extended to differential expressions of any order.

[40] In the theory of distributions, $u(x)$ usually stands for $\overline{u(x)}$ in (77). For s.a. differential expressions $\check{H}$ with real coefficients, $\overline{u(x)}$ in (77) can be equivalently replaced by $u(x)$, as for any even s.a. differential expression $\check{f}$, or for any odd s.a. expression $\check{f}$ with pure imaginary coefficients. Form (77) with $\overline{u(x)}$ is more convenient here because the following consideration is applicable to any mixed s.a. differential expression $\check{f}$ and because for (locally) square integrable $u(x)$, the integral in (77) becomes a scalar product $\left(u, \check{H}\varphi\right)$ in $L^2(a,b)$.

Lemma 5 *A function $\chi(x) \in D(a,b)$ is represented as*

$$\chi = \check{H}\phi\,,\ \phi \in D(a,b)\ ,$$

iff χ is orthogonal to solutions u of homogenous equation (74),

$$(u,\chi) = \int_a^b dx\overline{u(x)}\chi(x) = 0\,,\ \forall u:\ \check{H}u = 0\,, \tag{80}$$

which is evidently equivalent to the requirement that χ be orthogonal[41] *to fundamental solutions u_1 and u_2 of eq. (74), $(u_1,\chi) = (u_2,\chi) = 0$.*

The necessity immediately follows from equality (78) with $y = u$.

Sufficiency. Let $\chi \in D(a,b)$ and satisfy condition (80). For this χ, we take a specific solution ϕ of inhomogenous eq. (75) with $h = \chi$, $\check{H}\phi = \chi$, given by (76) with $c_1 = c_2 = 0$ and $\alpha = a$, $\beta = b$

$$\phi(x) = \frac{1}{W(u_1,u_2)}\left[u_1(x)\int_a^x d\xi u_2\chi + u_2(x)\int_x^b d\xi u_1\chi\right].$$

We can set $\alpha = a$ and $\beta = b$ even if the interval (a,b) is infinite because of a finite support of χ. Because u_1, u_2, and χ are smooth, the function ϕ is also smooth, $\phi \in C^\infty(a,b)$, and because of condition (80) and $\operatorname{supp}\chi(x) \subseteq [\gamma,\delta] \subset (a,b)$, we have $\phi = 0$ for $x < \gamma$ and $x > \delta$, i.e., $\phi \in D(a,b)$, which proves the lemma.

Lemma 6 *Any finite function $\varphi(x) \in D(a,b)$ can be represented as*

$$\varphi = c_1(\varphi)\varphi_1 + c_2(\varphi)\varphi_2 + \check{H}\phi\,,\ c_i(\varphi) = (u_i,\varphi)\ ,\ i = 1,2\,,$$

where u_1 and u_2 are fundamental solutions of homogenous equation (74), and φ_1, φ_2, and ϕ are some finite functions, φ_1, φ_2, $\phi \in D(a,b)$, such that

$$\left(u_i,\varphi_j\right) = \delta_{ij}\,,\ i,j = 1,2\,, \tag{81}$$

the functions, φ_1, φ_2 can be considered some fixed functions independent of φ.

We first prove the existence of a pair φ_1, φ_2 of finite functions with property (81) (although somebody may consider this evident). It is sufficient to show that there exists a pair ϕ_1, ϕ_2 of finite functions such that the matrix $A_{ij} = \left(u_i,\phi_j\right)$ is nonsingular, $\det A \neq 0$, and, therefore, has the inverse A^{-1}. Then the functions $\varphi_i = \left(A^{-1}\right)_{ji}\phi_j$ form the required pair. We now show qualitatively that the pair ϕ_1, ϕ_2 does exist. Let (α,β) be any finite interval in the initial interval (a,b). The restrictions of fundamental solutions u_1 and u_2 to this interval, i.e., u_1 and u_2 considered only for $x \in (\alpha,\beta)$, belong to $L^2(\alpha,\beta)$. The linear independence of fundamental solutions u_1 and u_2 implies that the matrix $U_{ij} = \int_\alpha^\beta dx\overline{u_i}u_j$, is nonsingular. Because $D(\alpha,\beta)$ is dense in $L^2(\alpha,\beta)$, we can find finite functions ϕ_1 and ϕ_2 that are arbitrarily close to the respective u_1 and u_2 on the interval (α,β). This implies that the matrix $A_{ij} = \int_\alpha^\beta dx\overline{u_i}\phi_j$, is also arbitrarily close to the matrix U, therefore, $\det A \neq 0$, and A is nonsingular. A reader can easily give a rigorous form to these qualitative arguments.

It then remains to note that the function $\varphi - c_1(\varphi)\varphi_1 - c_2(\varphi)\varphi_2$ satisfies the conditions of Lemma 5.

We can now prove a lemma generalizing the du-Boi-Reymond lemma.

[41] Although $u(x)$ is generally non-square-integrable, the symbol $(\,,)$ of a scalar product in (80) is proper because of a finite support of $\chi(x)$.

Lemma 7 *A locally integrable function $u(x)$ satisfies the condition (77)*

$$(u, H\varphi) = \int_a^b dx \overline{u} \check{H}\varphi = 0\,,\ \forall\varphi = D(a,b)\ ,$$

iff u is absolutely continuous in (a,b) together with its first derivative u' and satisfies homogenous equation (74) $\check{H}u = 0$. This means that any generalized solution of the homogenous equation is a usual solution.

As to sufficiency, it was already proved above based on eq. (78) (and actually repeats the proof of necessity in Lemma 5.

The necessity is proved using Lemma 6. For convenience of references, we let ϕ denote φ in (77), after which it becomes

$$\left(u, \check{H}\phi\right) = 0\,,\ \forall\phi = D(a,b)\ . \tag{82}$$

Let φ be an arbitrary finite function, $\varphi \in D(a,b)$. By Lemma 6, we have the representation

$$\varphi - (u_1, \varphi)\varphi_1 - (u_2, \varphi)\varphi_2 = \check{H}\phi$$

with some finite functions $\varphi_1, \varphi_2, \phi \in D(a,b)$, u_1 and u_2 are fundamental solutions of eq. (74). Substituting this representation of $\check{H}\phi$ in l.h.s. of (82) and appropriately rearranging it, we have

$$\begin{aligned}
\left(u, \check{H}\phi\right) &= (u, \varphi - (u_1, \varphi)\varphi_1 - (u_2, \varphi)\varphi_2) = (u, \varphi) - (u, \varphi_1)(u_1, \varphi) - (u, \varphi_2)(u_2, \varphi) \\
&= \left(u - \overline{(u, \varphi_1)}u_1 - \overline{(u, \varphi_2)}u_2, \varphi\right) = \int_\alpha^\beta dx \overline{(u - c_1 u_1 - c_2 u_2)}\varphi = 0\,,\ \forall\varphi = D(a,b)\ ,
\end{aligned}$$

where $c_i = (\varphi_i, u)$, $i = 1, 2$, are constants, which yields $u = c_1 u_1 + c_2 u_2$, representation (76) for a solution of eq. (74), and thus proves the lemma.

This lemma as well as the du-Boi-Rymond lemma are particular cases of the universal general theorem in the theory of distributions: the generalized solution of a homogenous differential equation of any order generated by a s.a. differential expression with smooth coefficients is a smooth function that is a usual solution of the same equation [29]. We only note that it is evident how the method for proving the above lemma, the method based on using the fundamental system of a homogenous equation, is extended to the general case.

As to the case of nonsmooth coefficients, a similar assertion on the generalized solutions of a homogenous equation also holds under the above-mentioned standard condition on the coefficients of the corresponding differential expression $\check{f}$ (64), (62), (63) and with an appropriate change of the space of finite functions in terms of which the generalized solution is defined. We recall that the standard conditions are that the coefficients f_{2k-1} and f_{2k} in (64), (62), (63) are k-time-differentiable and f_0 is locally integrable. Under these conditions, the homogenous equation $\check{f}u = 0$ is solvable and has a system $\{u_i\}^n$ of linearly independent fundamental solutions whose linear combination $u = \sum_{i=1}^n c_i u_i$ with arbitrary complex constants c_i, $i = 1, \ldots, n$, yields the general solution of the homogenous equation and in terms of which the general solution of the inhomogenous equation $\check{f}y = h$ is canonically expressed as a sum of a particular solution and the general solution of the homogenous equation; the constants c_i, $i = 1, \ldots, n$, are fixed by initial conditions on the respective u and y together with its $n-1$ derivatives at some inner point in (a,b) or at a regular end.

The only difference is that the space $D(a,b)$ of smooth finite functions that is universally suitable for differential expressions with smooth coefficients of any order is inappropriate in this case because $\check{f}\varphi$ is no longer smooth and has to be replaced for each differential expression of any order n by its own space $D_n(a,b)$ of functions φ with a compact support in (a,b) and absolutely continuous together with its $n-1$ derivatives

$$D_n(a,b) = \{\varphi : \varphi \in C^n(a,b)\ ,\ \operatorname{supp}\varphi \subseteq [\alpha,\beta] \subset (a,b)\}\ ; \tag{83}$$

of course, $D(a,b) \subset D_n(a,b)$. It is natural to keep the name "finite functions" for such functions. In the case of a regular end a where a solution of a homogenous equation has a finite limit together with its $n-1$ derivatives, the space $D_n(a,b)$ can be extended to functions vanishing at this regular end together with its $n-1$ derivatives. The same is true for a regular end b. It is easy to see that above Lemmas 5 and 6 are directly extended to such finite functions, and therefore, the extension Lemma 7 to s.a. differential expressions of any order also holds.

For even s.a. expressions, the corresponding assertion holds under the weakened above-mentioned conditions on the coefficients in terms of quasiderivatives, see [7, 8].

This result is the main ingredient in evaluating the adjoint of a preliminary symmetric operator associated with a given s.a. expression, see below.

3.4 Natural domain. Operator $\hat{f}^*$.

We are now ready to proceed to constructing s.a. operators in $L^2(a,b)$ associated with a given s.a. differential expression $\check{f}$ (64) based on the general theory of s.a. extensions of symmetric operators presented in the previous section. For simplicity, we consider the case of smooth coefficients which allows universally considering differential expressions and associated operators of any order. The results are naturally extended to the general case of nonsmooth coefficients under the above-mentioned conditions on the coefficients.

We begin with the so-called natural domain for a s.a. differential expression $\check{f}$ (64).

Let D_* be a subspace of square-integrable functions[42] ψ_* that are absolutely continuous[43] in (a,b) together with its $n-1$ derivatives and such that $\check{f}\psi_*$ is square-integrable as well as ψ_*:

$$D_* = \left\{\psi_* : \psi_*, \psi_*', \dots, \psi_*^{(n-1)} \text{ a.c. in } (a,b)\,;\ \psi_*,\ \check{f}\psi_* \in L^2(a,b)\right\}. \tag{84}$$

It is evident that D_* is the largest linear subspace in $L^2(a,b)$ on which a differential operator in $L^2(a,b)$ can be defined with the "rule of acting" given by $\check{f}$: the requirement that $\psi_*, \psi_*', \dots, \psi_*^{(n-1)}$ be absolutely continuous in (a,b) is necessary for $\check{f}\psi_*$ to have a sense of function, the requirement that ψ_* and $\check{f}\psi_*$ belong to $L^2(a,b)$ is necessary for ψ_* and $\check{f}\psi_*$ be the respective pre-image and image of an operator in $L^2(a,b)$ defined by $\check{f}$. We call the domain D_* (84) the natural domain for a s.a. differential expression $\check{f}$ (64) and let $\hat{f}^*$ denote the respective operator in $L^2(a,b)$ associated with the differential expression $\check{f}$ and defined on the natural domain D_*, such that

$$\hat{f}^* = \begin{cases} D_{f^*} = D_*\,, \\ \hat{f}^*\psi_* = \check{f}\psi_*\,. \end{cases} \tag{85}$$

[42]The expediency of this notation is justified below.

[43]When we say that some property of functions under consideration holds in (a,b), we mean that this property holds for any finite segment $[\alpha,\beta] \subset (a,b)$.

It is evident that the space $D(a,b)$ of finite smooth functions belongs to D_*, $D(a,b) \subset D_*$, and because $D(a,b)$ is dense in $L^2(a,b)$, $\overline{D(a,b)} = L^2(a,b)$, the domain D_* is all the more dense in $L^2(a,b)$, $\overline{D_*} = L^2(a,b)$, such that the operator $\hat{f}^*$ is densely defined.

As we already mentioned above in Comment 4 in the previous section, in the physical literature and even in some textbooks on quantum mechanics for physicists, s.a. differential expression (64) is identified with a s.a. operator in $L^2(a,b)$ without any reservation on its domain, and the spectrum and eigenfunctions of this operator are immediately looked for. Although its domain is not indicated, but actually, the natural domain for $\check{f}$ is implicitly meant by this domain: it is believed that the only requirements are the requirement of square integrability for the respective eigenfunctions of bound eigenstates and the requirement of local square integrability and the "normalization to δ-function" for (generalized) eigenfunctions of the continuous spectrum. In some cases, this appears sufficient, but sometimes, is not: possible situations are shortly described in Comment 4 in the previous section.

As we show later, to verify that $\hat{f}^*$ is s.a., it is sufficient to verify that it is symmetric, the necessary and sufficient conditions for which are that its sesquilinear asymmetry form ω_* or its quadratic asymmetry form Δ_* defined on its domain D_* respectively by, see (8), (9),

$$\omega_*(\chi_*, \psi_*) = \int_a^b dx \overline{\chi_*} \check{f} \psi_* - \int_a^b dx \psi_* \overline{\check{f} \chi_*}, \ \forall \chi_*, \psi_* \in D_*, \tag{86}$$

and

$$\Delta_*(\psi_*) = \int_a^b dx \overline{\psi_*} \check{f} \psi_* - \int_a^b dx \psi_* \overline{\check{f} \psi_*}, \ \forall \psi_* \in D_*, \tag{87}$$

vanish; because ω_* and Δ_* define each other, see the previous section, it is sufficient to do this for only one of this form.

We now show that the values of asymmetry forms ω_* (86) and Δ_* (87) are defined by the behavior of functions belonging to D_* near the ends a and b of the interval (a,b) because the both ω_* and Δ_* are determined by the boundary values of the respective sesquilinear form $[\chi_*, \psi_*]$ (70) and quadratic form $[\psi_*, \psi_*]$, its reduction to the diagonal, that are local forms in functions and its derivatives of order up to $n-1$. Really, by the integral Lagrange identity (71), we have

$$\omega_*(\chi_*, \psi_*) = [\chi_*, \psi_*]|_a^b = [\chi_*, \psi_*](b) - [\chi_*, \psi_*](a), \ \forall \chi_*, \psi_* \in D_*, \tag{88}$$

where, by definition,

$$[\chi_*, \psi_*](a) = \lim_{x \to a} [\chi_*, \psi_*], \ [\chi_*, \psi_*](b) = \lim_{x \to b} [\chi_*, \psi_*]; \tag{89}$$

the boundary values $[\chi_*, \psi_*](b)$ and $[\chi_*, \psi_*](a)$ of the form $[\chi_*, \psi_*]$ do exist for any $\chi_*, \psi_* \in D_*$ because the integrals in r.h.s. in (86) defining $\omega_*(\chi_*, \psi_*)$ exist. We note that the existence of limits (89) does not imply that the functions in D_* have the respective boundary values at a and b together with its $n-1$ derivatives; in general, these may not exist.

Similarly, for the quadratic asymmetry form Δ_* (87), we have

$$\Delta_*(\psi_*) = [\psi_*, \psi_*]|_a^b = [\psi_*, \psi_*](b) - [\psi_*, \psi_*](a), \tag{90}$$

where

$$[\psi_*, \psi_*](a) = \lim_{x \to a} [\psi_*, \psi_*], \ [\psi_*, \psi_*](b) = \lim_{x \to b} [\psi_*, \psi_*]. \tag{91}$$

We note that the boundary values (89) and (91) of local forms are independent in the following sense. Let we evaluate $[\chi_*, \psi_*](a)$ for some functions $\chi_*, \psi_* \in D_*$. For any function χ_*, there exists another function $\widetilde{\chi}_* \in D_*$ that coincides with χ_* near the end a and vanishes near the end b, more strictly $\widetilde{\chi}_* = \chi_*$, $a \leq x < \alpha < b$ and $\widetilde{\chi}_* = 0$, $\alpha < \beta < x \leq b$. In the case of a differential expression with differentiable coefficients[44], such a function can be obtained by multiplying χ_* by a smooth step-like function $\tilde{\theta}(x)$ equal to unity near $x = a$ and zero near $x = b$. In the case of an even differential expression with nondifferentiable coefficients, the multiplication by $\widetilde{\theta}$ in general makes $\widetilde{\chi_*}$ to leave the domain D_*, but the existence of functions $\widetilde{\chi}$ with the required properties can be proved [7, 8]. We then have $[\widetilde{\chi}_*, \psi_*](a) = [\chi_*, \psi_*](a)$ while $[\widetilde{\chi}_*, \psi_*](b) = 0$. The same is true for the end b. It follows that the conditions of vanishing the asymmetry form ω_* with an arbitrary first argument, i.e., the condition $\omega_*(\chi_*, \psi_*) = 0$, $\forall \chi_* \in D_*$, is equivalent to the condition of separately vanishing boundary values (89), i.e., to the boundary conditions

$$[\psi_*, \psi_*](a) = [\psi_*, \psi_*](b) = 0\,, \ \forall \psi_* \in D_*\,. \tag{92}$$

It is evident that we can interchange the first and second arguments χ_* and ψ_* in the above consideration.

All the above-said is true for boundary values (91). In particular, the condition $\Delta_*(\psi_*) = 0$, $\forall \psi_* \in D_*$, for an operator $\hat{f}^*$ associated with a differential expression $\check{f}$ is equivalent to the boundary conditions (92).

It follows that an answer to the question of whether the operator $\hat{f}^*$ (85) is symmetric, and therefore s.a., or not, is defined by possible boundary values (89) and (91) for the respective asymmetry forms ω_* and Δ_* for all functions in D_*, namely, whether they vanish identically or not. We shortly discuss the possibility to answer the question. For definiteness, we speak about boundary values (91). The natural domain D_* (84) can be defined as the space of square-intergrable solutions ψ_* of the differential equation

$$\check{f}\psi_* = \chi_*\,, \ \forall \chi_* \in L^2(a, b)\ . \tag{93}$$

Therefore, boundary values (91) can be evaluated by analyzing the behavior of the general solution ψ_* of eq. (93) near the ends a and b of the interval (a, b) with the additional condition that ψ_* must be square integrable up to the ends.

If we succeeded in proving that boundary values (91) vanish for all functions in D_*, we thus prove that the operator $\hat{f}^*$ (85) associated with a given differential expression $\check{f}$ and defined on the natural domain D_* (84) is s.a.. We show later that it is a unique s.a. operator associated with $\check{f}$. Therefore, it seems evident that the first thing we should do is to attempt to prove that boundary values (91) of the quadratic local form $[\psi_*, \psi_*]$ vanish for all functions ψ_* in the natural domain D_* (84). But if we can indicate a function $\psi_* \in D_*$ such that, for example, $[\psi_*, \psi_*](a) \neq 0$, we thus prove that the operator $\hat{f}^*$ (85) is nonsymmetric and, all the more, non-s.a..

In general, the set of possible boundary values (91) depends on the type of the interval (a, b), namely, whether it is a whole axis $\mathbb{R}^1$, or a semiaxis, or a finite interval, and on the behavior of the coefficients of $\check{f}$ as $x \to a$ and $x \to b$. We illustrate possible situations by simple examples related to differential expression $\check{H}$ (65).

[44]This is a short name for a differential expression with coefficients satisfying the standard differentiability conditions, in particular, with smooth coefficients.

Let $(a,b)=(-\infty,\infty)=\mathbb{R}^1$, and let $\check{f}=\check{H}$ given by (65) with the zero potential, $V=0$. We conventionally let $\check{H}_0$ denote this differential expression,

$$\check{H}_0=-\frac{d^2}{dx^2}\,, \tag{94}$$

it is identified with the Hamiltonian of a free nonrelativistic particle moving along the real axis $\mathbb{R}^1$. The natural domain D_{0*} for $\check{H}_0$ is

$$D_{0*}=\left\{\psi_*:\ \psi_*,\ \psi_*'\ \text{a.c. in}\ \mathbb{R}^1;\ \psi_*,\ \psi_*''\in L^2(\mathbb{R}^1)\right\}\,. \tag{95}$$

As we already mentioned above, $\psi_*\in L^2(\mathbb{R}^1)$ does not imply that $\psi_*\to 0$ as $x\to\pm\infty$. Therefore, the proof of the self-adjointness (actually, the symmetricity) of the free Hamiltonian based on the opposite assertion in some textbooks for physicists is incorrect. But it can be shown, and we show this later, that $\psi_*\in D_{0*}$ (95) implies that $\psi_*,\psi_*'\to 0$ as $x\to\pm\infty$, and therefore, the quadratic local form $[\psi_*,\psi_*]=-\left[\overline{\psi_*}\psi_*'-\overline{\psi_*'}\psi_*\right]$ for $\check{H}_0$, see (72) with $\chi_*=\psi_*$, vanishes at infinities, $[\psi_*,\psi_*]\to 0\,,\ x\to\pm\infty$, i.e., boundary values (91) vanish for all ψ_* in this case. It follows that the operator $\hat{H}_0$ (we conventionally omit the upperscript $*$) associated with the differential expression $\check{H}_0$ and defined on the natural domain, the free Hamiltonian, is really s.a., which we know from textbooks. As we show later, the same is true for the potential $V(x)=x^2$, we then deal with the differential expression $\check{H}=-d^2/dx^2+x^2$, which is identified with the Hamiltonian for a quantum oscillator: the same local form $[\psi_*,\psi_*]$ vanishes at infinities also in this case. This implies that the operator $\hat{H}$ associated with this differential expression $\check{H}=-d^2/dx^2+x^2$ and defined on the natural domain

$$D_*=\left\{\psi_*:\ \psi_*,\psi_*'\ \text{a.c. in}\ \mathbb{R}^1\,;\ \psi_*,-\psi_*''+x^2\psi_*\in L^2(\mathbb{R}^1)\right\}\,.$$

is s.a., which we also know from textbooks.

But let now $V(x)$ be a rather exotic potential rapidly going to $-\infty$ as $x\to\pm\infty$, for example, let $V=-x^4$, such that the "Hamiltonian" is $\check{H}=-d^2/dx^2-x^4$. Let ψ_* be a square-integrable smooth function that exponentially vanishes as $x\to-\infty$ and such that

$$\psi_*=\frac{1}{x}\exp\left(\frac{i}{3}x^3\right)\,,\ x>N>0\,.$$

It is easy to verify that ψ_* belongs to the natural domain D_* for this $\check{H}$:

$$-\psi_*''-x^4\psi_*=-\frac{2}{x^3}\exp\left(\frac{i}{3}x^3\right)\,,\ x>N\,,$$

and is square-integrable at $+\infty$, as well as ψ_*, while the left end, $-\infty$, is evidently safe. It is also easy to evaluate the form $[\psi_*,\psi_*]$ for $x>N$, it is $[\psi_*,\psi_*]=-2i$. It follows that for this function, the boundary value $[\psi_*,\psi_*](+\infty)=-2i\neq 0$, which implies that the operator $\hat{H}^*$ associated with the differential expression $\check{H}=-d^2/dx^2-x^4$ and defined on the natural domain

$$D_*=\left\{\psi_*:\ \psi_*,\psi_*'\ \text{a.c. in}\ \mathbb{R}^1;\psi_*,-\psi_*''-x^4\psi_*\in L^2(\mathbb{R}^1)\right\}$$

is non-s.a., and even nonsymmetric,and,therefore, it cannot be considered a quantum-mechanical Hamiltonian for a particle in the potential field $V=-x^4$. The correct Hamiltonian in this

case requires an additional specification. We only note in advance that this is possible, but nonuniquely. It is also interesting that the spectrum of such a Hamiltonian is discrete, although it may seem unexpected at the first glance.

If the interval (a, b) is a semiaxis, for example, the positive semiaxis $(0, \infty)$, and the left end $a = 0$ is regular, then ψ_*, ψ'_* are continuous up to this end and can take arbitrary complex values, which implies that $[\psi_*, \psi_*](0) = -\left[\overline{\psi_*(0)}\psi'_*(0) - \overline{\psi'_*(0)}\psi_*(0)\right]$ can also take arbitrary nonzero imaginary values and, therefore, the operator $\hat{H}^*$ is not s.a..

An important remark concerning real quantum mechanics is in order here.

In physics, the differential expressions like (65) on the positive semiaxis usually have a three-dimensional origin. Their standard source is a problem of a space motion of a quantum particle in spherically symmetric or axially symmetric fields.

Let we consider a space motion, for example, the scattering or bound states, of a nonrelativistic spinless particle in a spherically symmetric field. The quantum states of the particle are described by wave function $\psi(\mathbf{r})$, $\mathbf{r}$ is the radius-vector, $\psi(\mathbf{r}) \in L^2(R^3)$, and the motion is governed by the "Hamiltonian" $\mathbf{H} = -\Delta + V(r)$, where Δ is the Laplacian, $V(r)$ is a potential, and $r = |\mathbf{r}|$ (the appropriate units are assumed, in particular, $\hbar = 1$). The problem is usually solved by separating the variables $\mathbf{r} \to r, \theta, \varphi$, where θ, φ are spherical angles. When passing from the three-dimensional wave function $\psi(\mathbf{r})$ to its partial waves $u_l(r, \theta, \varphi) = u_l(r)Y_{lm}(\theta, \varphi)$, where Y_{lm} are spherical harmonics, $\psi(\mathbf{r}) = \sum_{l=0}^{\infty} (2l+1)u_l(r)Y_{lm}(\theta, \varphi)$, the differential expressions like (65) naturally arise as the so called radial "Hamiltonians" $\check{H}_l$ for the radial motion with the angular momentum $l = 0, 1, ...$:

$$\check{H}_l = -\frac{d^2}{dr^2} + V_l(r)\,, \tag{96}$$

where the partial potential $V_l(r)$ is

$$V_l(r) = V(r) + \frac{l(l+1)}{r^2} \tag{97}$$

and includes the so-called centrifugal term $l(l+1)/r^2$. The radial motion is described in terms of the radial wave functions $\psi_l(r) \in L^2(0, \infty)$ that differ from the partial amplitudes $u_l(r)$ by the factor r, $\psi_l(r) = ru_l(r)$, which is essential. If the initial three-dimensional potential $V(r)$ is nonsingular at the origin or have rather weak singularity (we do not define an admissible singularity for $V(r)$ at $r = 0$ more precisely here, see [19], the natural domain for the three-dimensional Hamiltonian $\mathbf{H}$ consists of functions $\psi_*(\mathbf{r})$ that are sufficiently regular in the neighborhood of the origin, such that the partial amplitudes $u_l(r)$ are finite at $r = 0$ and, therefore, the radial wave functions $\psi_l(r)$ must vanish at $r = 0$. In this setting, the natural domain D_{*l} for $\check{H}_l$ is reduced to a domain D_l that differs form D_{*l} by the additional boundary condition $\psi_l(0) = 0$. This boundary condition is the well-known conventional condition in physics for the radial wave-functions. If, in addition, $[\psi_l, \psi_l](\infty) = 0$, which holds if $V(r) \to 0$ as $r \to 0$, as we show later, then the operator $\hat{H}_l$ associated with the differential expression $\check{H}_l$ (96), (97) and defined on the domain D_l is a s.a. operator and can be considered a quantum-mechanical observable that we know from textbooks. To be true, the zero boundary condition at $r = 0$ for the radial wave functions is critical only for the s-wave, $l = 0$, because for $l = 1, 2, \ldots$ the natural domain D_{*l} coincides with D_l.

These arguments fail if the potential is strongly singular, for example, in the cases where $V = -\alpha/r^2$, $\alpha > -\frac{1}{4}$, or $V = -\alpha/r^\beta$, $\alpha > 0$, $\beta > 2$, and where the so-called phenomenon of "fall to the center" occurs.

A similar consideration can be carried out for a motion of a particle in an axially symmetric potential field $V(\rho)$, ρ is the distance to the axis, with the same conclusion for the partial radial Hamiltonians

$$\check{H}_m = -\frac{d^2}{d\rho^2} + V_m(\rho) \ ,$$

where the partial potential is

$$V_m(\rho) = V(\rho) + \frac{m^2}{\rho^2} \, ,$$

and $m = 0, 1, \ldots$ is the projection of the angular momentum to the axis. The reason is that the radial wave functions $\psi_m(\rho) \in L^2(0, \infty)$ differ from the original partial amplitudes $u_m(\rho)$ square integrable with the measure $\rho d\rho$ by the factor $\rho^{1/2}$, $\psi_m(\rho) = \rho^{1/2} u_m(\rho)$, and if the initial potential $V(\rho)$ is not too singular, the natural domain for $\check{H}_m$ is supplied by the additional boundary condition $\psi_m(0) = 0$.

If an interval (a, b) is finite and one of its ends a and b or the both are regular, then one of the boundary values (91) or the both can be nonzero, and, therefore, the operator $\hat{H}^*$ associated with the differential expression $\check{H}$ and defined on the natural domain is non-s.a. in this case. For example, this assertion holds for the differential expression (94), the "Hamiltonian" for a free particle on a finite interval of the real axis. The physical reason for this is evident: a particle can "escape" from or enter the interval through the ends, which results in the nonunitarity of evolution. Only additional physical arguments preventing these possibilities by additional boundary conditions that make the asymmetry form Δ_* (87) to be zero result in the self-adjointness of the real Hamiltonian $\hat{H}_0$ associated with the differential expression $\check{H}_0$. The most known s.a. boundary conditions are $\psi(a) = \psi(b) = 0$, which corresponds to a particle in an "infinite potential well", and the periodic boundary conditions $\psi(a) = \psi(b)$, $\psi'(a) = \psi'(b)$ (the latter condition is usually hidden in textbooks), which corresponds to "quantization in a box" conventionally used in statistical physics.

3.5 Initial symmetric operator and its adjoint. Deficiency indices.

We now return to the general consideration. Because the operator $\hat{f}^*$ (85) associated with the s.a. differential expression $\check{f}$ (64) and defined on the natural domain D_* is generally non-s.a., we proceed to the general programme of constructing s.a. operators presented in the previous section. In the case of differential operators in $L^2(a, b)$, it is mainly based on a possibility to represent their asymmetry forms ω_* and Δ_* in terms of (asymptotic) boundary values of the local form $[\cdot, \cdot]$ (70) similar to the respective (88), (89), and (90), (91).

As the first step, we must define a symmetric operator in $L^2(a, b)$ associated with a given s.a. differential expression $\check{f}$ of order n. In the case of smooth coefficients, it is natural to take the subspace $D(a, b)$ of smooth functions, $D(a, b) \subset L^2(a, b)$, for a domain of such an operator and thus to start with a symmetric operator $\hat{f}^{(0)}$ defined in $L^2(a, b)$ by

$$\hat{f}^{(0)} : \begin{cases} D_{f^{(0)}} = D(a, b) \ , \\ \hat{f}^{(0)}\varphi = \check{f}\varphi \, , \ \forall \varphi \in D(a, b) \ . \end{cases} \tag{98}$$

It is evident that $\check{f}\varphi \in L^2(a,b)$ as well as φ because of a finite support of φ. It is also evident that $\hat{f}^{(0)}$ is symmetric because it is densely defined, $\overline{D(a,b)} = L^2(a,b)$, and the equality

$$\left(\phi, \hat{f}^{(0)}\varphi\right) = \left(\phi, \hat{f}^{(0)}\varphi\right), \ \forall\varphi, \phi \in D_{f^{(0)}} = D(a,b)$$

holds because it coincides with eq. (57) $\left(\phi, \check{f}\varphi\right) = \left(\check{f}\phi, \varphi\right)$ for the s.a. $\check{f} = \check{f}^*$, the latter equality is simply the manifestation of the self-adjointness of $\check{f}$ as a differential expression, see also eq. (79) with $y = \phi$. We emphasize once more that because of the self-adjointness of $\check{f}$ as a differential expression, $\hat{f}^{(0)}$ is generally only a symmetric, but not s.a., operator in $L^2(a,b)$.

The second step is evaluating the adjoint $\left(\hat{f}^{(0)}\right)^+$ by solving the defining equation

$$\left(\psi_*, \hat{f}^{(0)}\varphi\right) - (\chi_*, \varphi) = 0, \ \forall\varphi \in D_{f^{(0)}}$$

for a pair of vectors $\psi_* \in D_{\left(f^{(0)}\right)^+} \subset L^2(a,b)$ and $\chi_* = \left(\hat{f}^{(0)}\right)^+ \psi_* \in L^2(a,b)$, see subsec.2.1. In our case, this is the equation

$$\int_a^b dx\overline{\psi_*}\check{f}\varphi - \int_a^b dx\overline{\chi_*}\varphi = 0, \ \forall\varphi \in D(a,b), \tag{99}$$

for a pair of square-integrable functions ψ_* and χ_*. We assert that the adjoint $\left(\hat{f}^{(0)}\right)^+$ coincides with the above-introduced operator $\hat{f}^*$ (85), $\left(\hat{f}^{(0)}\right)^+ = \hat{f}^*$, in particular, its domain $D_{\left(f^{(0)}\right)^+}$ is the natural domain D_* (84). In other words, we assert that functions $\psi_* \in L^2(a,b)$ and $\chi_* \in L^2(a,b)$ solve eq. (99) iff ψ_* is absolutely continuous in (a,b) together with its derivatives of order up to $n-1$ and $\chi_* = \check{f}\psi_*$.

Sufficiency is evident because of eq. (79) with $y = \psi_*$.

Necessity is proved as follows. Let $\psi_* \in L^2(a,b)$ and $\chi_* \in L^2(a,b)$ solve eq. (99), and let $\widetilde{\psi}_*$ be some solution of the inhomogenous differential equation $\check{f}\,\widetilde{\psi}_* = \chi_*$. Such a function certainly exists because the square integrability of $\chi_*(x)$ implies its local integrability in (a,b); in addition, $\tilde{\psi}_*$ is absolutely continuous in (a,b) together with its derivatives of order up to $n-1$. We then have

$$\int_a^b dx\,\overline{\chi_*}\varphi = \int_a^b dx\varphi\,\overline{\check{f}\tilde{\psi}_*} = \int_a^b dx\overline{\tilde{\psi}_*}\,\check{f}\varphi$$

because of the same eq. (79) with $y = \tilde{\psi}_*$, and the defining equation (99) becomes

$$\int_a^b dx\,\overline{u}\check{f}\varphi = 0, \ \forall\varphi \in D(a,b),$$

where $u = \psi_* - \tilde{\psi}_*$.

By the above-cited distribution theory theorem on the generalized solution of the homogeneous equation $\check{f}u = 0$, it follows that $u = \sum_{i=1}^n c_i u_i$, where $\{u_i\}_1^n$, is a fundamental system of this homogeneous equation, and we finally obtain that $\psi_* = \tilde{\psi}_* + \sum_{i=1}^n c_i u_i$, which implies, that ψ_* is absolutely continuous in (a,b) together with its derivatives of order up to $n-1$ and $\chi_* = \check{f}\psi_*$. This completes the proof of the above assertion.

This assertion is evidently extended to the general case of nonsmooth coefficients under the standard conditions on the coefficients of a differential expression with a change of the domain $D_{f^{(0)}}$ of the initial symmetric operator $\hat{f}^{(0)}$ from the space $D(a,b)$ of finite smooth functions to the space $D_n(a,b)$ (83) of finite functions. For even s.a. expressions, the requirements on the coefficients can be weakened up to the similar conditions on the quasiderivatives, see [7, 8].

The main conclusion is that in any case, the adjoint $\left(\hat{f}^{(0)}\right)^+$ of the initial symmetric operator $\hat{f}^{(0)}$ associated with a s.a. differential expression $\check{f}$ (64) is given by the same differential expression $\check{f}$ and defined on the natural domain. Under the the standard conditions on the coefficients of $\check{f}$, the natural domain D_* is given by (84) and the adjoint $\left(\hat{f}^{(0)}\right)^+$ coincides with the operator $\hat{f}^*$ (85). For even s.a. differential expression, the condition of absolute continuity for derivatives can be weakened to the same condition on quasiderivatives.

Therefore, the asymmetry forms ω_* and Δ_* of the adjoint $\left(f^{(0)}\right)^+$ coincide with the respective forms ω_* (86) and Δ_* (87) and are represented respectively by (88), (89) and (90), (91) in terms of boundary values of the local form $[\cdot,\cdot]$ (70).

According to the general theory, if the adjoint $\left(f^{(0)}\right)^+$ appears to be symmetric, which is equivalent to identically vanishing boundary values (89) and (91), then $\left(f^{(0)}\right)^+$ is s.a., the initial symmetric operator $\hat{f}^{(0)}$ is essentially s.a. and its unique s.a. extension is its closure $\overline{\hat{f}^{(0)}} = \hat{f}$ coinciding with its adjoint $\left(\hat{f}^{(0)}\right)^+$. This justifies our preliminary statement that if the operator $\hat{f}^*$ (85) associated with a s.a. differential expression $\check{f}$ (64) and defined on the natural domain D_* (84) is symmetric, then it is s.a. and is a unique s.a. operator associated with a given differential expression.

But according to the previous discussion, the adjoint $\left(\hat{f}^{(0)}\right)^+ = \hat{f}^*$ is generally nonsymmetric and we must continue our programme of constructing s.a. operators associated with a given differential expression $\check{f}$ by extending the initial symmetric operator $\hat{f}^{(0)}$ and restricting the adjoint[45] $\left(\hat{f}^{(0)}\right)^+ = \hat{f}^*$. According to this programme, the next step is evaluating the deficient subspaces D_+ and D_- of the initial symmetric operator $\hat{f}^{(0)}$,

$$D_\pm = \left\{\psi_\pm \in D_* : \ \hat{f}^*\psi_\pm = \pm i\kappa\psi_\pm\right\} ,$$

and its deficiency indices m_+ and m_-, $m_\pm = \dim D_\pm$. In our case, D_+ and D_- are the spaces of square-integrable solutions ψ_+ and ψ_- of the respective homogeneous differential equations

$$\check{f}\psi_\pm = i\kappa\psi_\pm \, , \tag{100}$$

where κ is an arbitrary, but fixed, dimensional parameter whose dimension is the dimension of $\check{f}$.

We must find the complete systems $\{e_{+,k}\}_1^{m_+}$ and $\{e_{-,k}\}_1^{m_-}$ of linearly independent square-integrable solutions of respective eqs. (100):

$$\check{f}e_{+,k} = i\kappa e_{+,k} \, , \ k = 1,\ldots,m_+ \, , \ \check{f}e_{-,k} = -i\kappa e_{-,k} \, , \ k = 1,\ldots,m_- \, ; \tag{101}$$

[45]We note once again that an additional specification of a "Hamiltonian" $\check{H}$ by some boundary conditions for wave functions (which is a standard practice in physics) is actually a self-adjoint restriction of $\hat{H}^*$ when it becomes clear that the Hamiltonian under consideration is non-self-adjoint on the natural domain.

for the future, it is convenient to orthonormalize them,

$$(e_{+,k}, e_{+,l}) = \delta_{kl}\ ,\ k,l = 1,\ldots,m_+\ ,\ (e_{-,k}, e_{-,l}) = \delta_{kl}\ ,\ k,l = 1,\ldots,m_-\ , \tag{102}$$

then $\{e_{+,k}\}_1^{m_+}$ and $\{e_{-,k}\}_1^{m_-}$ form the orthobasises in the respective D_+ and D_-,

$$\psi_+ = \sum_{k=1}^{m_+} c_{+,k} e_{+,k}\ ,\ c_{+,k} = \left(e_{+,k}, \psi_+\right)\ ;\ \psi_- = \sum_{k=1}^{m_+} c_{-,k} e_{-,k}\ ,\ c_{-,k} = \left(e_{-,k}, \psi_-\right)\ .$$

As to possible values of deficiency indices, the following remarks of the general nature can be useful.

We first note that the deficiency indices m_+ and m_- of a symmetric ordinary differential operator of order n are always finite and do not exceed n: for a differential expression $\check{f}$ of order n, the whole number of linearly independent solutions, fundamental solutions $u_{\pm i}(x)$, of each of homogenous equations (100), is equal to n, the additional requirement of square integrability of solutions can only reduce this number, such that we generally have the restriction $0 \le m_+, m_- \le n$.

As is clear from the above discussion of the operator $\hat{f}^*$, the deficiency indices depend both on the type of the interval (a,b) and on the type of its ends a and b, whether they are regular or singular. If some end, a or b, is regular, the general solution of each of eqs. (100) is square integrable at this end, and the square integrability of ψ_+ and ψ_- is thus defined by their square integrability at singular ends.

It follows that in the case where the interval (a,b) is finite and the both its ends are regular, we have $m_+ = m_- = n$ for any symmetric operator $\hat{f}^{(0)}$ of order n. According to the main theorem in the previous section, this implies that there is a n^2-parameter $U(n)$-family of s.a. operators associated with a given differential expression $\check{f}$ of order n. For example, the differential expression (38) generates a one-parameter $U(1)$-family of s.a. operators each of which can be considered the quantum-mechanical momentum of a particle on a finite interval of the real axis (we already know this fact from the previous section), while the differential expression (94) generates a four-parameter $U(2)$-family of s.a. operators each of which can be considered the quantum-mechanical energy of a free particle on a finite interval. This means that for a particle on a finite interval, an explicitly s.a. differential expression does not yet define uniquely a quantum-mechanical observable, and a further specification of the observable is required. We show later that this specification is achieved by s.a. boundary conditions on the wave functions in the domain of the observable. The optimistic point of the conclusion is that s.a. operators associated with any s.a. differential expression do exist in this case.

As to the case where one or both ends are singular, the situation is not so optimistic in general. In particular, it is different for even s.a. differential expressions with real coefficients and for odd s.a. differential expressions with pure imaginary coefficients, all the more for mixed differential expressions.

For even s.a. differential expressions $\check{f}$, the deficiency indices of the associated symmetric operator $\hat{f}^{(0)}$ are always equal, $m_+ = m_- = m$, independently of the type of an interval and its ends. Really, because of the real coefficients of $\check{f}$, any square-integrable solution ψ_+ of eq. (100) is assigned a square-integrable solution $\psi_- = \overline{\psi_+}$, while the linear independence of solutions preserves under complex conjugation. In particular, for basis vectors $e_{+,k}$ in D_+ and $e_{-,k}$ in D_- defined by (101), we can take complex conjugated functions such that $e_{-,k} = \overline{e_{+,k}},\ k = 1,...,m$. Therefore, any even s.a. expression always generates at least one s.a. operator in $L^2(a,b)$

in contrast to odd s.a. differential expressions, as we already know from the previous section by the example of the first-order differential expression $\check{p}$ (38). In particular, for any interval (a, b), the energy of a nonrelativistic particle associated with a differential expression $\check{H}$ (65) can always be defined as a quantum-mechanical observable, although in general nonuniquely.

The last two assertions on deficiency indices concern symmetric operators associated with even s.a. expressions[46], see [7, 8]; for brevity, we call them even symmetric operators. These assertions are based on the notion of the dimension of a linear space modulo its subspace, on the boundary properties of the functions in the domain of the closure of an even symmetric operator at a regular end, on first von Neumann formula (4), and on second von Neumann formula (23) and the remark to the second von Neumann theorem on the relation between the deficiency indices of a symmetric operator and its symmetric extension.

Let L be some linear space, and let M be its subspace, $M \subset L$. We consider the factor space L/M, or the space L modulo the subspace M, that is a linear space whose vectors are equivalent classes of vectors in L with respect to the equivalence relation where two vectors $\xi \in L$ and $\eta \in L$ are considered equivalent if their difference belongs to M, $\xi - \eta \in M$. The dimension of the factor space L/M is denoted by $\dim_M L$ and is called the dimension of L modulo M. Linearly independent vectors $\xi_1, \xi_2, \ldots, \xi_k \in L$ are called linearly independent modulo M if none of their nontrivial linear combinations $\sum_{i=1}^{k} c_i \xi_i$ belongs to M: $\sum_{i=1}^{k} c_i \xi_i \in M \Longrightarrow \forall c_i = 0$. If $\dim_M L = n$, then the maximum number of vectors in L linearly independent modulo M is equal to n, such that $k \leq n$. Let a space L be a direct sum of two its subspaces L_1 and L_2, $L = L_1 \dot{+} L_2$, then its dimension is a sum of the dimensions of the subspaces, $\dim L = \dim L_1 + \dim L_2$, and $\dim_{L_1} L = \dim L_2$ and $\dim_{L_2} L = \dim L_1$.

We discuss the closures of symmetric operators $\hat{f}^{(0)}$ a bit later, and here, we only need one preliminary remark on this subject. Let $\hat{f}^{(0)}$ be an <u>even</u> symmetric operator of order n with a regular end, let it be a, let $\hat{f}$ be its closure, $\hat{f} = \overline{\hat{f}^{(0)}}$, with a domain D_f. It appears that at a regular end, the functions in D_f vanish together with their $n-1$ quasiderivatives: $\psi_f \in D_f \Longrightarrow \psi_f^{[k]}(a) = 0$, $k = 0, \ldots, n-1$.

After this retreat, we return to the deficiency indices of even symmetric operators.

If one of the ends of an interval (a, b) is regular, let it be a, while the second, b, is singular, the deficiency indices of even symmetric operator $\hat{f}^{(0)}$ of order n, being equal, $m_+ = m_- = m$, and bounded from above, $m \leq n$, are also bounded from below by $n/2$, such that the double-sided restriction

$$\frac{n}{2} \leq m \leq n \tag{103}$$

holds. In particular, the symmetric operator $\hat{H}^{(0)}$ associated with the differential expression $\check{H}$ (65) for the energy of a nonrelativistic particle on a semiaxis $(0, \infty)$ in a potential field V, where V is regular at $x = 0$, can have the deficiency indices $m = 1$ and $m = 2$ in dependence on the behavior of V at infinity, but not zero. This implies that the quantum-mechanical Hamiltonian for such a particle cannot be defined uniquely as a s.a. operator in $L^2(0, \infty)$ without additional arguments. This fact is known since Weyl [23], where the cases $m = 1$ and $m = 2$ were respectively called the case of a "limit point" and the case of "limit circle" due to a method of embedded circles used by Weyl.

To prove the lower bound, we turn to the representation of the domain D_* of the adjoint

[46] Although it is quite probable that similar assertions hold for any s.a. differential expressions, perhaps under some additional conditions for the coefficients.

$\left(\hat{f}^{(0)}\right)^{+}=\hat{f}^{*}$ as a direct sum of D_f, D_+ and D_-, $D_*=D_f+D_++D_-$, according to first von Neumann formula (4). This formula implies that the maximum number of functions in D_* linearly independent modulo D_f is equal to $2m$ because

$$\dim_{D_f} D_* = \dim(D_+ + D_-) = \dim D_+ + \dim D_- = 2m\,.$$

If we prove that there exists a set $\{\psi_{*l}\}_1^n$ of functions in D_* linearly independent modulo D_f, we would have $n \leq 2m$, which is required. But we know that the functions ψ_* in D_* together with their quasiderivatives $\psi_*^{[k]}$ of order up to $n-1$ are finite at a regular end and can take arbitrary values. Therefore, in our case of the regular end a, there exists a set $\{\psi_{*l}\}_1^n$ of linearly independent functions such that the matrix A, $A_l^k=\psi_{*l}^{[k]}(a)$, is nonsingular, $\det A \neq 0$. We assert that these functions are also linearly independent modulo D_f . Really, let $\sum_l c_l\psi_{*l}=\psi\in D_f$. Then by the above remark, $\psi^{[k]}(a)=0$, or $\sum_l c_l\psi_{*l}^{[k]}(a)=\sum_l A_l^k c_l=0$, whence it follows that all $c_l=0$, $l=1,..,n$, because of the nonsingularity of the matrix A, which completes the proof.

In the case where the both ends a and b of an interval (a,b) are singular, the evaluation of deficiency indices is reduced to the case of one regular and one singular end by a specific symmetric restriction of an initial symmetric operator $\hat{f}^{(0)}$ and a comparison of the respective closures of the restriction and $\hat{f}^{(0)}$ itself.

Let $\check{f}$ be an even s.a. differential expression of order n on an interval (a,b) with the both singular ends, let $\hat{f}^{(0)}$ be a symmetric operator in $L^2\left(a,b\right)$ associated with $\check{f}$, let $m_+=m_-=m$ be its deficiency indices, and let $\hat{f}$ be its closure, $\hat{f}=\overline{\hat{f}^{(0)}}$. Let c be an intermediate point in the interval (a,b), $a<c<b$, such that $(a,b)=(ac)\cup(cb)$. We note that the Hilbert space $L^2\left(a,b\right)$ is a direct sum of the Hilbert spaces $L^2\left(a,c\right)$ and $L^2\left(c,b\right)$, $L^2\left(a,b\right)=L^2\left(a,c\right)\oplus L^2\left(c,b\right)$.

We consider the s.a. restrictions $\check{f}_-$ and $\check{f}_+$ of the initial s.a. expression $\check{f}$ to the respective intervals (a,c) and (c,b); the end c for both differential expressions $\check{f}_-$ and $\check{f}_+$ is evidently regular. Let $\hat{f}_-^{(0)}$ and $\hat{f}_+^{(0)}$ be the symmetric operators in the respective $L^2\left(a,c\right)$ and $L^2\left(c,b\right)$ associated with the respective s.a. expressions $\check{f}_-$ and $\check{f}_+$ of order n and defined on the respective domains $D\left(a,c\right)\subset L^2\left(a,c\right)$ and $D\left(c,b\right)\subset L^2\left(c,b\right)$; let their deficiency indices be respectively $m_+^{(-)}=m_-^{(-)}=m^{(-)}$ and $m_+^{(+)}=m_-^{(+)}=m^{(+)}$, and let $\hat{f}_-$ and $\hat{f}_+$ be their closures in the respective $L^2\left(a,c\right)$ and $L^2\left(c,b\right)$, $\hat{f}_-=\overline{\hat{f}_-^{(0)}}$ and $\hat{f}_+=\overline{\hat{f}_+^{(0)}}$, with the respective domains $D_{f_-}\subset L^2\left(a,c\right)$ and $D_{f_+}\subset L^2\left(c,b\right)$. Because the end c is regular for the both f_- and f_+, the functions in the both domains D_{f_-} and D_{f_+} vanish at the end c together with their derivatives of order up to $n-1$.

We now consider a new symmetric operator $\hat{f}_c^{(0)}$ in $L^2\left(a,b\right)$ associated with the initial differential expression $\check{f}$ and defined on the domain $D_{f_c^{(0)}}$ that is a direct sum of $D\left(a,c\right)$ and $D\left(c,b\right)$, $D_{f_c^{(0)}}=D\left(a,c\right)\oplus D\left(c,b\right)$. It is evident that $\overline{D_{f_c^{(0)}}}=L^2\left(a,b\right)$ and $D_{f_c^{(0)}}\subset D\left(a,b\right)=D_{f^{(0)}}$, such that $\hat{f}_c^{(0)}$ is a symmetric operator in $L^2\left(a,b\right)$ that is a specific symmetric restriction of the symmetric operator $\hat{f}^{(0)}$, $\hat{f}_c^{(0)}\subset\hat{f}^{(0)}$. Let its deficiency indices be $m_{c+}=m_{c-}=m_c$, and let $\hat{f}_c$ be its closure in $L^2\left(a,b\right)$, $\hat{f}_c=\overline{\hat{f}_c^{(0)}}$, it is evident that $\hat{f}_c\subset\hat{f}$.

The crucial remark is that $\hat{f}_c^{(0)}$ is a direct sum of the operators $\hat{f}_-^{(0)}$ and $\hat{f}_+^{(0)}$, $\hat{f}_c^{(0)}=\hat{f}_-^{(0)}\dot{+}\hat{f}_+^{(0)}$. It follows, first, that its deficiency indices are the sums of the deficiency indices of the summands, i.e.,

$$m_c=m^{(-)}+m^{(+)}\,, \tag{104}$$

and, second, that its closure $\hat{f}_c$ is a direct sum of the closures $\hat{f}_-$ and $\hat{f}_+$, $\hat{f}_c = \hat{f}_- + \hat{f}_+$, which implies that $\hat{f}_c$ is the restriction of $\hat{f}$ to the domain $D_{f_c} \subset D_f$ that differs from D_f by the only additional condition on the functions $\psi \in D_f$ that $\psi^{[k]}(c) = 0$, $k = 0, 1, \ldots, n-1$, which in turn implies that there exist exactly n, and not more, linearly independent functions in D_f that do not satisfy this condition and are linearly independent modulo D_{f_c}, i.e.,

$$\dim_{D_{f_c}} D_f \; = n\,. \tag{105}$$

On the other hand, the second von Neumann theorem is applicable to $\hat{f}$ as a nontrivial symmetric extension of $\hat{f}_c^{(0)}$. According to this theorem, namely to second von Neumann formula (23) and to the remark ii) to the theorem, the dimension of D_f modulo D_{f_c} is equal to the difference of the deficiency indices of $\hat{f}_c^{(0)}$ and $\hat{f}^{(0)}$[47],

$$\dim_{D_{f_c}} D_f \; = m_c - m\,. \tag{106}$$

The comparison of (104), (105), and (106) yields the relation

$$m = m^{(+)} + m^{(-)} - n \tag{107}$$

between the deficiency indices of $\hat{f}^{(0)}$ and $\hat{f}_-^{(0)}$, $\hat{f}_+^{(0)}$. We note that because $n/2 \leq m^{(-)}$, $m^{(+)} \leq n$, this relation is compatible with the general restriction on the deficiency indices of $\hat{f}^{(0)}$, $0 \leq m \leq n$. It is known that in the case where the both ends are singular, the deficiency indices can take any value from 0 to n [7, 8].

Let we evaluate the deficient subspace D_+ and D_- and the respective deficiency indices m_+ and m_- of an initial symmetric operator $\hat{f}^{(0)}$ associated with a given s.a. differential expression $\check{f}$.

By the main theorem in the previous section, we know that three possibilities for the s.a. extensions of $\hat{f}^{(0)}$ can occur.

Let the deficiency indices be different, $m_+ \neq m_-$ which can happen only for odd or mixed s.a. expressions with at least one singular end. In this case, there exist no s.a. extensions of $\hat{f}^{(0)}$, i.e., there is no s.a. differential operators associated with a given s.a. differential expression $\check{f}$.

Let the both deficiency indices be equal to zero, $m_+ = m_- = 0$, for even s.a. differential expressions, this can happen only if the both ends are singular[48]. In this case, the initial symmetric operator $\hat{f}^{(0)}$ is essentially s.a., and its unique s.a. extension is it closure $\hat{f}$ that coincides with its adjoint $\left(\hat{f}^{(0)}\right)^+ = \hat{f}^*$. In other words, there is only one s.a. differential operator in $L^2(a,b)$ associated with a given differential expression $\check{f}$. As we already mentioned above, this fact can become clear without evaluating the deficient subspaces and deficient indices if the asymmetry form Δ_*, or ω_*, is easily evaluated and appears to be zero.

Let the both deficiency indices be different from zero and equal, $m_+ = m_- = m > 0$, which is always the case if the both ends are regular. In this case, there exists an m^2-parameter family of s.a. extensions of $\hat{f}^{(0)}$. In other words, there is an $U(m)$-family $\left\{\hat{f}_U\right\}$ of s.a. operators $\hat{f}_U$, $U \in U(m)$, the group, associated with a given differential expression $\check{f}$, and the problem of their proper and convenient, if possible, specification arises.

[47] We recall that the deficiency indices of a symmetric operator and its closure coincide.

[48] A natural hypothesis is that the same is true for any s.a. differential expression.

3.6 Specification of self-adjoint extensions in terms of deficient subspaces.

Two simple preliminary remarks are useful. First, any s.a. extension $\hat{f}_U$ of an initial symmetric operator $\hat{f}^{(0)}$ is simultaneously a s.a. extension of its closure $\hat{f}$ with a domain D_f and a symmetric restriction of the adjoint $\left(\hat{f}^{(0)}\right)^+ = \hat{f}^*$ with a domain D_*. All these operators are given by the same initial differential expression $\check{f}$, but defined on different domains such that $D_f \subset D_{f_U} \subset D_*$, where D_{f_U} is the domain of $\hat{f}_U$. Therefore, a specification of a s.a. operator $\hat{f}_U$ is completely defined by a specification of its domain D_{f_U}, second, because the deficiency indices of the symmetric operator $\hat{f}^{(0)}$ of any finite order n are finite, $m < \infty$, the isometries $\hat{U} : D_+ \to D_-$ defining the s.a. extensions $\hat{f}_U$ in the main theorem are defined by $m \times m$ unitary matrices $U = \|U_{lk}\|$, $l,k = 1,2,\ldots,m$, $U^+ = U^{-1}$.

The main theorem furnishes the two ways of specification.

The first way is based on formulas (33), (34) for D_{f_U} and requires the knowledge of the domain D_f of the closure $\hat{f}$ apart from the deficient subspaces D_+ and D_-. The domain D_f is defined by formula (13) with the appropriate change of notation $D_{\bar{f}} \to D_f$, $D_{f^+} \to D_*$, $\underline{\psi} \to \psi$, and $\xi_* \to \psi_*$, or equivalently by formulas (15) or (16) with the additional change of notation $\xi_z, \xi_{\bar{z}} \to \psi_+, \psi_-$ (100) and $e_{z,k}$, $e_{\bar{z},k} \to e_{+,k}$, $e_{-,k}$ (101) with $m_+ = m_- = m$.

We use the definition of D_f by (13): $D_f = \{\psi \in D_* : \omega_*(\psi_*, \psi) = 0\,,\ \forall \psi_* \in D_*\}$, where $\omega_*(\psi_*, \psi)$ is given by (88), $\omega_*(\psi_*, \psi) = [\psi_*, \psi]|_a^b$ in terms of boundary values (89) of a local bilinear form $[\psi_*, \psi]$ which certainly exist. Taking the above remarks (after formula (91)) on the independence of these boundary values, we can reduce the condition $\omega_*(\psi_*, \psi) = 0$, $\forall \psi_* \in D_*$, to the independent boundary conditions

$$[\psi_*, \psi](a) = [\psi_*, \psi](b) = 0\,,\ \forall \psi_* \in D_*. \tag{108}$$

We formulate the result as a lemma.

Lemma 8 *The domain D_f of the closure $\hat{f}$ of a symmetric operator $\hat{f}^{\,(0)}$ associated with a s.a. differential expression $\check{f}$ is specified by two boundary conditions (108) and is given by*

$$D_f = \{\psi \in D_* :\ [\psi_*, \psi](a) = 0\,,\ [\psi_*, \psi](b) = 0\,,\ \forall \psi_* \in D_*\}\,. \tag{109}$$

In some cases, boundary conditions (108) in (109) can be explicitly represented in terms of boundary conditions on the functions ψ and their (quasi)derivatives of order up to $n-1$, where n is the order of $\check{f}$, at the end a and/or b. For example, let $\check{f}$ be an even differential expression of order n on an interval (a,b) and let the left end a be regular. Then ψ and its quasiderivatives of order up to $n-1$ have finite values $\psi^{[k]}(a)$, $k = 0,1,\ldots,n-1$, at the end a, as well as any $\psi_* \in D_*$, and the condition $[\psi_*, \psi](a) = 0$ becomes

$$\sum_{k=0}^{\frac{n}{2}-1} \left(\overline{\psi_*^{[k]}(a)}\psi^{[n-k-1]}(a) - \overline{\psi_*^{[n-k-1]}(a)}\psi^{[k]}(a) \right) = 0\,,$$

see (73). Because $\psi_*^{[k]}(a)$, $k = 0,1,\ldots,n-1$, can take arbitrary values, the boundary condition $[\psi_*, \psi](a) = 0$, $\forall \psi_* \in D_*$, reduces to zero boundary conditions $\psi^{[k]}(a) = 0\,,\ k = 0,1,\ldots,n-1$

for functions $\psi \in D_f$ and their quasiderivatives at the left regular end a. The same is true for the regular end b.

We thus obtain that, in the presence of regular ends, a more explicit form can be given to Lemma 8.

Lemma 9 *If $\check{f}$ is an even s.a. differential expression of order n with both regular ends, then the domain D_f is given by*

$$D_f = \left\{ \psi(x) \in D_* : \psi^{[k]}(a) = \psi^{[k]}(b) = 0\,,\ k = 0, 1, \ldots, n-1 \right\}, \tag{110}$$

if only one end, let it be a, regular, then the domain D_f is given by

$$D_f = \left\{ \psi(x) \in D_* : \psi^{[k]}(a) = 0,\ k = 0, 1, \ldots, n-1; [\psi_*, \psi](b) = 0,\ \forall \psi_* \in D_* \right\}. \tag{111}$$

It is evident that this result can be extended to any s.a. differential expression $\check{f}$ with differentiable coefficients and regular ends with the change of quasiderivatives to usual derivatives if a local form $[\chi_*, \psi_*]$ in functions and their derivatives up to order $n-1$ is nondegenerate at regular ends.

As an illustration, we consider two simple s.a. differential expressions $\check{p}$ (38) and $\check{H}_0$ (94) on a finite interval $[0, l]$, the both ends of which are evidently regular. The domain D_p of the closure $\hat{p}$ of the initial symmetric operator $\hat{p}^{(0)}$ with the domain $D_{p^{(0)}} = D(0, l)$ is given by[49]

$$D_p = \left\{ \psi : \psi \text{ a.c. on } [0, l]\ ;\ \psi,\ \psi' \in L^2(0, l)\ ;\ \psi(0) = \psi(l) = 0 \right\}, \tag{112}$$

we already know this result from the previous section, see (50), while the domain D_{H_0} of the closure $\hat{H}_0$ of the initial symmetric operator $\hat{H}_0^{(0)}$, $D_{H_0^{(0)}} = D(0, l)$, is given by

$$D_{H_0} = \left\{ \psi :\ \psi,\ \psi' \text{ a.c. on } [0, l]\,;\ \psi,\ \psi'' \in L^2(0, l)\,;\ \psi(0) = \psi(l) = \psi'(0) = \psi'(l) = 0 \right\}. \tag{113}$$

We note that the same domain evidently has the symmetric operator $\hat{H}$ associated with the s.a. differential expression $\check{H}$ (65) in the case where the potential V is bounded $|V(x)| < c < \infty$. If V is nonbounded but locally integrable, the domain D_H for the corresponding $\hat{H}$ is changed in comparison with D_{H_0} (112) by the only replacement of the condition $\psi'' \in L^2(0, l)$ by the condition $-\psi'' + V\psi \in L^2(0, l)$.

We also note that both $\hat{H}_0$ and $\hat{H}$ are evidently symmetric, but not s.a., because of the additional zero boundary conditions on the derivatives.

After the specification of the domain D_f of the closure $\hat{f}$, we can formulate a theorem describing all s.a. operators associated with a given s.a. differential expression $\check{f}$.

This theorem is a paraphrase of the main theorem in the part related to formulas (33), (36).

Theorem 10 *The set of all s.a. differential operators associated with a given s.a. differential expression $\check{f}$ in the case where the initial symmetric operator $\hat{f}^{(0)}$ has nonzero equal deficiency indices $m_+ = m_- = m > 0$ is the m^2-parameter $U(m)$-family $\left\{ \hat{f}_U \right\}$ parametrized by elements*

[49] The condition $\psi \in L_2(a, b)$ is not independent; it is automatically fulfilled in view of the first condition of the absolute continuity of ψ on the whole $[0, l]$; we give it for completeness.

of the unitary group $U(m)$, $U\in U(m)$. Namely, each s.a. operator $\hat{f}_U$ is in one-to-one correspondence with a unitary matrix $U=\|U_{lk}\|$, $l,k=1,2,\ldots,m$, $U^{+}=U^{-1}$, and is given by

$$\hat{f}_U:\left\{\begin{array}{l} D_{f_U}=\left\{\psi_U=\psi+\sum_{k=1}^{m}c_k\left[e_{+,k}+\sum_{l=1}^{m}U_{lk}e_{-,k}\right],\,\forall\psi\in D_f,\ \forall c_k\in\mathbb{C}\right\},\\ \hat{f}\psi_U=\check{f}\psi_U\,,\end{array}\right. \tag{114}$$

where D_f is the domain of the closure $\hat{f}$ of $\hat{f}^{\ (0)}$ specified by (109), or (110), or (111), $\{e_{+,k}\}^m$ and $\{e_{-,k}\}^m$ are orthobasises in the respective deficient subspaces D_+ and D_- defined by (100),(101), and (102). In the case of an even differential expression with real coefficients, we can take $e_{-,k}=\overline{e_{+,k}}$.

As an illustration, we consider the simple examples of differential expressions $\check{p}$ (38) and $\check{H}_0$ (94) on a finite interval $[0,l]$. Both ends are regular, which implies that the deficiency indices (m_+,m_-) are the respective $(1,1)$, i.e., $m=1$, and $(2,2)$, i.e., $m=2$. Therefore, for the differential expressions $\check{p}$, we have a one-parameter $U(1)$-family $\{\hat{p}_\theta\}$ of associated s.a. operators $\hat{p}_U=\hat{p}_\theta$ because in this case, $U=e^{i\theta}$, $0\leq\theta\leq2\pi$, $0\backsim2\pi$; this family is completely described in the previous section. For the differential expression $\check{H}_0$, we have a four-parameter $U(2)$-family $\left\{\hat{H}_{0,U}\right\}$ of associated s.a. operators $\hat{H}_{0,U}$, $U\in U(2)$, which we describe below.

To simplify the description, it is convenient to choose the dimensional parameter κ in (100) to be $\kappa=2(\pi/l)^2$. For the orthobasis vectors in the deficient two-dimensional subspaces D_+ and D_-, we can take the respective functions

$$\begin{aligned} e_{+,1} &= \sigma\exp\rho\,,\ e_{+,2}=\sigma\exp(\pi-\rho)\ ,\ \rho=(1-i)\,\pi\frac{x}{l}\,,\\ e_{-,1} &= \overline{e_{+,1}}\,,\ \ e_{-,2}=\overline{e_{+,2}}\,,\ \sigma=\left(e^{2\pi}-1\right)^{-1/2}(2\pi/l)^{1/2}\ , \end{aligned} \tag{115}$$

where σ is a normalization factor. In view of (112), the s.a. operator $\hat{H}_{0U}$ associated with the differential expression $\check{H}_0$ is then given by[50]

$$\hat{H}_{0U}:\left\{\begin{array}{l} D_{H_{0U}}=\Big\{\psi_U=\psi+\sum_{j=1}^{2}c_je_{U,j}\,:\,\psi,\psi'\,\text{a.c. on}\,[0,l]\,;\,\psi,\psi''\in L^2(0,l)\ ,\,\psi(0)\\ =\psi(l)=\psi'(0)=\psi'(l)=0\,;\ e_{U,j}=e_{+,j}+\sum_{k=1}^{2}U_{kj}\overline{e_{+,k}}\,,\ j=1,2;\ \forall c_j\in\mathbb{C}\Big\}\,,\\ \hat{H}_{0U}\psi_U=-\psi_U''\,,\end{array}\right. \tag{116}$$

where $U=\|U_{kj}\|$, $k,j=1,2$, is a unitary matrix.

The normalization factor σ in $e_{+,1}$, $e_{+,2}$ (115) can be absorbed in c_1, c_2 and is irrelevant.

As we already mentioned above, this specification of the domain $D_{H_{0U}}$ by specifying the functions ψ_U in $D_{H_{0U}}$ as a sum of functions $\psi\in D_{H_0}$ and an arbitrary linear combination of vectors $e_{U,j}$, $j=1,2$, that are the basis vectors in the two-dimensional subspace $\left(D_++\hat{U}D_+\right)$ seems inconvenient for spectral analysis of $\hat{H}_{0U}$ and is unaccustomed in physics where we used to appeal to (s.a.) boundary conditions for functions ψ_U in $D_{H_{0U}}$, these conditions are relations between the boundary values of the functions and their first derivatives, without mentioning the domain D_{H_0}.

[50] We change the notation of indices in (116) in comparison with (113) to avoid a confusion with the index l and the symbol l for the right end of the interval.

The main observation is that according to formula

$$\psi_U(x) = \psi(x) + \sum_{k=1}^{2} c_j e_{U,j}(x) \ , \tag{117}$$

the four boundary values of the absolutely continuous functions ψ_U and ψ'_U are defined by the only second term in r.h.s. in (117) because of the zero boundary values of ψ and ψ', namely, by the certain boundary values of $e_{U,j}$ and $e'_{U,j}$ and only two arbitrary constants c_1 and c_2, which result in two relations between the boundary values of ψ_U and ψ'_U, the relations defined by the unitary matrix U. To demonstrate this fact, it is convenient to proceed in terms of two-columns and 2×2 matrices. Formula (117) yields

$$\begin{pmatrix} \psi_U(0) \\ \psi'_U(0) \end{pmatrix} = E_U(0) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} , \ \begin{pmatrix} \psi_U(l) \\ \psi'_U(l) \end{pmatrix} = E_U(l) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} . \tag{118}$$

where the 2×2 matrices $E_U(0) = \|E_{U,kj}(0)\|$ and $E_U(l) = \|E_{U,kj}(l)\|$ are given by

$$E_{U,kj}(0) = e_{U,j}^{(k-1)}(0) \ , \ E_{U,kj}(l) = e_{U,j}^{(k-1)}(l) \ .$$

It turns out that the rank of the rectangular 4×2 matrix $\begin{pmatrix} E_U(0) \\ E_U(l) \end{pmatrix}$ is maximal and equal to 2. Therefore, we could express constants c_1 and c_2 in terms of $\psi_U(0), \dots, \psi'_U(l)$ from some two relations in (118), then substitute the obtained expressions in the remaining two relations and thus obtain two linear relations between the boundary values of functions in $D_{H_{0U}}$ and their first derivatives that are defined by the matrix U. But it is more convenient to proceed as follows. We multiply the first and the second relation in (118) by the respective matrices $E_U^+(0)\,\mathcal{E}$ and $E_U^+(l)\,\mathcal{E}$, where the matrix $\mathcal{E}{=}\sigma^2/i$ and obtain that

$$E_U^+(0)\,\mathcal{E} \begin{pmatrix} \psi_U(0) \\ \psi'_U(0) \end{pmatrix} = E_U^+(0)\,\mathcal{E} E_U(0) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} ,$$
$$E_U^+(l)\,\mathcal{E} \begin{pmatrix} \psi_U(l) \\ \psi'_U(l) \end{pmatrix} = E_U^+(l)\,\mathcal{E} E_U(l) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} .$$

The crucial remark is that the matrix

$$R = E_U^+(l)\,\mathcal{E} E_U(l) - E_U^+(0)\,\mathcal{E} E_U(0)$$

is the null matrix: taking (88), (89), and (72) for $\check{f} = \check{H}_0$,

$$[\chi_*, \psi_*] = \sum_{k,j=1}^{2} \overline{\chi_*^{(k-1)}(x)} \mathcal{E}_{kj} \psi_*^{(j-1)}(x) \ ,$$

into account, it is easy to see that matrix elements of R are

$$R_{kj} = [e_{U,k}, e_{U,j}]|_0^l = \omega_*(e_{U,k}, e_{U,j}) = 0$$

because the reduction of the sesquilinear antisymmetric form ω_* to $D_{H_{0U}}$ is equal to zero. It follows that

$$E_U^+(l)\,\mathcal{E} \begin{pmatrix} \psi_U(l) \\ \psi'_U(l) \end{pmatrix} - E_U^+(0)\,\mathcal{E} \begin{pmatrix} \psi_U(0) \\ \psi'_U(0) \end{pmatrix} = 0 \, , \tag{119}$$

which is equivalent to

$$[e_{U,j}, \psi_U]|_0^l = 0\,,\ j = 1, 2\,. \tag{120}$$

Relations (119), (120) are the boundary conditions specifying the s.a. extension $\hat{H}_{0U}$, i.e., the s.a. boundary conditions. It is clear how the representation (117) for $\psi_U \in D_{H_{0U}}$ is restored from boundary conditions (119), (120) by reversing the above procedure. It is also clear how this consideration is generalized to s.a. operators associated with even differential expressions of any order in the case where both ends are regular.

3.7 Specification of self-adjoint extensions in terms of self-adjoint boundary conditions

The second alternative way of the specification of s.a. differential operators $\hat{f}_U$ in $L^2(a,b)$ associated with a given s.a. differential expression $\check{f}$, the operators that are s.a. extensions of the initial symmetric operator $\hat{f}^{(0)}$, is based on formulas (35), (37) in the main theorem and formulas (88), (89) for the asymmetry form ω_*. It avoids the evaluation of the domain $\hat{f} = \overline{\hat{f}^{(0)}}$ of the closure D_f and directly leads to the specification of the s.a. operators $\hat{f}_U$ in terms of s.a. boundary conditions. A corresponding theorem is alternative to Theorem 4; it is a paraphrase of the main theorem in the part related to formulas (35), (37) with due regard to formulas (88), (89) and the appropriate change of notation in (37): $\xi_U \to \psi_U$. For brevity, we do not repeat the first general assertion and the explanation of symbols that are common to the both theorems. We also introduce the abbreviated notation $e_{U,k}$ for the basis functions $e_{+,k} + \sum_{l=1}^m U_{lk} e_{-,k}$ in the subspace $\left(D_+ + \hat{U}D_+\right) \subset D_{f_U} \subset D_*$.

Theorem 11 *Each s.a. operator $\hat{f}_U$ in $L^2(a,b)$ associated with a given s.a. differential expression $\check{f}$ is given by*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{\psi_U \in D_* :\ [e_{U,k}, \psi_U]|_a^b = 0\right\}, \\ \hat{f}_U \psi_U = \check{f}\psi_U\,, \end{cases} \tag{121}$$

where $e_{U,k} = e_{+,k} + \sum_{l=1}^m U_{lk} e_{-,l}\,.$

We make two remarks on Theorem 11. First, this theorem explicitly specifies $\hat{f}_U$ as a restriction of the adjoint $\hat{f}^*$ to the domain D_{f_U} defined by s.a. boundary conditions. These boundary conditions considered as additional linear equations for functions $\psi_* \in D_*$ are linearly independent. Really, let the relation

$$\sum_{k=1}^m c_k \left[e_{U,k}, \psi_*\right]\Big|_a^b = 0\,,\ \forall\psi_* \in D_*\,,$$

holds, with some constants c_k. This relation is equivalent to $[\psi_*, \sum_{k=1}^m \overline{c_k} e_{U,k}]|_a^b = 0$ and by Lemma 8, see (109), implies that $\sum_{k=1}^m \overline{c_k} e_{U,k} \in D_f$, which is possible only if all $c_k = 0$, $k = 1, \dots, m$, because $D_f \cap \left(D_+ + \hat{U}D_+\right) = \{0\}$, or, in other words, because the functions $e_{U,k}$

are linearly independent modulo D_f. Second, the basis functions $e_{U,k}$ in $\left(D_+ + \hat{U}D_+\right)$ belong to D_{f_U}, therefore, the relation

$$[e_{U,k}, e_{U,l}]|_a^b = 0\,,\ k,l = 1,\ldots,m, \tag{122}$$

holds; its particular realization for $\check{f} = \check{H}_0$ with $m = 2$ was already encountered above.

In some particular cases, boundary conditions (121) in Theorem 11 become explicit boundary conditions in terms of boundary values of functions and their (quasi)derivatives. We here present two such cases. The first is the case of even s.a. differential expressions of order n on a finite interval (a,b) with the both regular ends, the case where the functions in D_* and their quasiderivatives of order up to $n-1$ have finite boundary values and where the deficiency indices are maximum, $m_+ = m_- = n$. By formula (73), the s.a. boundary conditions become

$$[e_{U,k}, \psi_U]|_a^b = -\sum_{l=0}^{\frac{n}{2}-1}\left[\overline{e_{U,k}^{[l]}}\psi_U^{[n-l-1]} - \overline{e_{U,k}^{[n-l-1]}}\psi_U^{[l]}\right]\Bigg|_a^b = 0\,,\ k = 1,\ldots,n\,,$$

or, shifting up the summation index by unity,

$$\sum_{l,m=1}^{n}\left[\overline{e_{U,k}^{[l-1]}\left(b\right)}\mathcal{E}_{lm}\psi_U^{[m-1]}\left(b\right) - \overline{e_{U,k}^{[l-1]}\left(a\right)}\mathcal{E}_{lm}\psi_U^{[m-1]}\left(a\right)\right] = 0\,,\ k = 1,\ldots,n\,, \tag{123}$$

where

$$\mathcal{E}_{lm} = \delta_{l,n+1-m}\epsilon\left(l - \frac{n+1}{2}\right)\,,\ l,m = 1,\ldots,n\,, \tag{124}$$

and $\epsilon\left(x\right)$ is the well-known odd step function, $\epsilon\left(-x\right) = -\epsilon\left(x\right)$ and $\epsilon\left(x\right) = 1$ for $x > 0$. Boundary conditions (123) can be conveniently represented in condensed terms of the matrix $\mathcal{E} = \|\mathcal{E}_{lm}\|$, where $\mathcal{E}_{lm}$ are given by (124), the two $n\times n$ matrices of boundary values of the basis functions $e_{U,k}$ and their quasiderivatives,

$$\begin{aligned} &E_U\left(a\right) = \|E_{U,lk}\left(a\right)\|\,,\ E_{U,lk}\left(a\right) = e_{U,k}^{[l-1]}\left(a\right)\,,\\ &E_U\left(b\right) = \|E_{U,lk}\left(b\right)\|\,,\ E_{U,lk}\left(b\right) = e_{U,k}^{[l-1]}\left(b\right)\,,\ l,k = 1,\ldots,n\,, \end{aligned} \tag{125}$$

and the two n-columns of boundary values of functions and their quasiderivatives,

$$\Psi_U\left(a\right) = \begin{pmatrix} \psi_U\left(a\right)\\ \psi_U^{[1]}\left(a\right)\\ \vdots\\ \psi_U^{[n]}\left(a\right)\end{pmatrix}\,,\ \Psi_U\left(b\right) = \begin{pmatrix} \psi_U\left(b\right)\\ \psi_U^{[1]}\left(b\right)\\ \vdots\\ \psi_U^{[n]}\left(b\right)\end{pmatrix}\,. \tag{126}$$

Their realization for $\check{f} = \check{H}_0$ was already encountered above. It seems useful to give a separate version of Theorem 11 for this case in the introduced condensed notation.

Theorem 12 *Any s.a. operator $\hat{f}_U$ in $L^2\left(a,b\right)$ associated with an even s.a. differential expression $\check{f}$ of order n with the both regular ends is given by*

$$\hat{f}_U : \left\{\begin{array}{l} D_{f_U} = \left\{\psi_U \in D_* :\ E_U^+\left(b\right)\mathcal{E}\Psi\left(b\right) - E_U^+\left(a\right)\mathcal{E}\Psi\left(a\right) = 0\right\}\,,\\ \hat{f}_U\psi_U = \check{f}\psi_U\,,\end{array}\right. \tag{127}$$

where the matrices $\mathcal{E}$, $E_U\left(a\right)$, $E_U\left(b\right)$ and the columns $\Psi\left(a\right),\Psi\left(b\right)$ are given by the respective (124), (125), and (126).

The modified version of the two remarks to Theorem 11 in this case is

1) s.a. boundary conditions (127) are linearly independent, which is equivalent to the property of the matrices $E_U(a)$ and $E_U(b)$ that the $2n\times n$ matrix $\mathbb{E}$ has the maximum rank,

$$\mathbb{E}=\left(\begin{array}{c}E_U(a)\\ E_U(b)\end{array}\right),\ \mathrm{rank}\mathbb{E}=n\,; \tag{128}$$

really the above given proof of the linear independence of boundary conditions was based on the property that $\sum_{k=1}^{m}c_k e_{U,k}\in D_f\Longrightarrow c_k=0,\ k=1,...,m$, but in our case where $m=n$, in view of Lemma 9, formula (110), this is equivalent to the property that

$$\sum_{k=1}^{n}e_{U,k}^{[l-1]}(a)\,c_k=0\,,\ \sum_{k=1}^{n}e_{U,k}^{[l-1]}(b)\,c_k=0\,,\ l=1,...,n\Longrightarrow c_k=0,\ k=1,...,n\,;$$

2) relation (122) is written as

$$E_U^{+}(b)\,\mathcal{E}E_U(b)-E_U^{+}(a)\,\mathcal{E}E_U(a)=0\,. \tag{129}$$

Of course, in practical applications, the condensed notation requires decoding, see below an example of the differential expression $\check{H}_0$.

We also note that matrices $E_U(a)$ and $E_U(b)$ with a given unitary matrix U depend on the choice of the dimensional parameter κ in (100) and on the choice of the orthobasises $\{e_{+,k}\}_1^n$ and $\{e_{-,k}\}_1^n$ in the respective deficient subspaces D_+ and D_-. For example, if we change the orthobasises,

$$\{e_{+,k}\}_1^n\to\left\{\widetilde{e}_{+,k}=\sum_{l=1}^{n}V_{+lk}e_{+,l}\right\}_1^n,\ \{e_{-,k}\}_1^n\to\left\{\widetilde{e}_{-,k}=\sum_{l=1}^{n}V_{-lk}e_{-,l}\right\}_1^n,$$

where matrices $V_\pm$ are unitary, and it is not obligatory that $V_-=\overline{V_+}$, then the matrix U for the same s.a. extension is replaced according to the rule $U\to\tilde{U}=V_-^{-1}UV_+$.

Again , as after Lemma 9, we can add that a similar theorem holds for any s.a. differential expression $\check{f}$ of any order with differentiable coefficients and the both regular ends with the change of quasiderivatives by usual derivatives if boundary values (89) are finite forms in the boundary values of functions and their derivatives.

As an illustration, we consider our simple examples of differential expressions $\check{p}$ (38) and $\check{H}_0$ (94) on a finite interval $[0,l]$ and compare the descriptions of the respective one-parameter set of s.a. operators $\hat{p}_U$, $U\in U(1)$, and four-parameter set of s.a. operators $\hat{H}_{0U}$, $U\in U(2)$, according to Theorem 10 and to Theorem 12 respectively. For the operators $\hat{p}_U$, this was already done in the previous section, and it was demonstrated that the two descriptions are equivalent. As to $\hat{H}_{0U}$, we must preliminarily evaluate the domain D_{0*} of $\hat{H}_0^*$. This is a natural domain for $\check{H}_0$ and is evidently given by (95) with the only change $\mathbb{R}^1\to[0,l]$. After this, any s.a. operator $\hat{H}_{0U}$ is given by

$$\hat{H}_{0U}:\left\{\begin{array}{l}D_{H_{0U}}=\{\psi_U:\psi_U,\,\psi_U'\text{ a.c. on }[0,l]\,;\ \psi_U,\,\psi_U''\in L^2(0,l)\ ;\\ E_U^{+}(l)\,\mathcal{E}\Psi_U(l)=E_U^{+}(0)\,\mathcal{E}\Psi_U(0)\}\ ,\\ \hat{H}_{0U}\psi_U=-\psi_U''\,,\end{array}\right.$$

where $\mathcal{E}$ and $E_U(l)$, $E_U(0)$ are the matrices given by the respective (124) and (125) with $n=2$ and the usual first derivatives of the basis vectors $e_{U,k}$ given by (115), (116), while the two-columns $\Psi_U(0)$ and $\Psi_U(l)$ are

$$\Psi_U(0) = \begin{pmatrix} \psi_U(0) \\ \psi_U'(0) \end{pmatrix},\ \Psi_U(l) = \begin{pmatrix} \psi_U(l) \\ \psi_U'(l) \end{pmatrix},$$

see (126) with $n=2$, all these were already encountered above. If we compare this description of $\hat{H}_{0U}$ according to Theorem 12 with that obtained from Theorem 10 and given by (119), we find that they are identical.

It is interesting to give examples of s.a. operators $\hat{H}_{0U}$ associated with the differential expression $\check{H}_0$ (94) on $[0,l]$ and corresponding to particular choices of the unitary matrix U. Each of them is a candidate to the quantum mechanical Hamiltonian for a free particle on the interval $[0,l]$.

Choosing $U=I$, the unit matrix, we obtain the Hamiltonian $\hat{H}_{0I}$ specified by the s.a. boundary conditions that being decoded and presented in conventional form[51] looks rather exotic:

$$\begin{aligned} \psi(l) &= -\cosh\pi\,\psi(0) - \frac{l}{\pi}\sinh\pi\,\psi'(0)\ , \\ \psi'(l) &= -\frac{\pi}{l}\sinh\pi\,\psi(0) - \cosh\pi\,\psi'(0)\ , \end{aligned} \tag{130}$$

Choosing $U=-I$, we obtain the Hamiltonian $\hat{H}_{0\,-I}$ specified by the well-known s.a. boundary conditions

$$\psi(0) = \psi(l) = 0 \tag{131}$$

corresponding to a particle in an infinite potential well.

Choosing $U=iI$, we obtain the Hamiltonian $\hat{H}_{0\,iI}$ specified by the s.a. boundary conditions

$$\psi'(0) = \psi'(l) = 0\,. \tag{132}$$

Choosing $U = -\frac{1}{2}\left[(1-i)\,I + (1+i)\,\sigma^1\right]$, we obtain the Hamiltonian $\hat{H}_{0U}$ specified by the periodic boundary conditions[52]

$$\psi(0) = \psi(l)\ ,\ \psi'(0) = \psi'(l)\ , \tag{133}$$

conventionally adopted in statistical physics when quantizing an ideal gas in a box.

The second case where the s.a. boundary conditions in Theorem 11 become explicit in terms of boundary values of functions and their (quasi)derivatives of order up to $n-1$ is the case of even s.a. differential expression $\check{f}$ of order n with one regular and one singular end for which the associated initial symmetric operator $\hat{f}^{(0)}$ has minimum possible deficiency indices[53] $m_+ = m_- = n/2$, see (103). This follows from some general assertion on differential symmetric operators.

[51]When writing boundary conditions with a specific U separately, we conventionally omit the subscript U in the notation of the respective functions.

[52]To be true, in this case we actually solve the inverse problem of finding a proper U for periodic boundary conditions.

[53]We recall that the deficiency indices are always equal in the case of an even s.a. differential expression.

Lemma 13 *Let $\hat{f}^{(0)}$ be a symmetric operator associated with an even s.a. differential expression $\check{f}$ of order n on an interval (a,b) with the regular end a and the singular end b, and let the deficiency indices of $\hat{f}^{(0)}$ be $m_+ = m_- = n/2$. Then the equality*

$$[\chi_*, \psi_*](b) = 0\,,\ \forall \chi_*, \psi_* \in D_*\,, \tag{134}$$

where D_* is the domain of the adjoint $\hat{f}^* = \left(\hat{f}^{(0)}\right)^+$ holds. If the end a is singular while the end b is regular, then b in (134) is changed to a.

We show later that conversely, if the boundary values $[\chi_*, \psi_*](b)$ vanish for all $\chi_*, \psi_* \in D_*$, the deficiency indices of $\hat{f}^{(0)}$ are minimum, $m_+ = m_- = n/2$.

The proof of the Lemma is based on the arguments already known and used above in the proof of the independence of boundary values (89) and in the proof of the lower bound in (103). Therefore, we don't repeat them and only formulate two initial assertions following from the conditions of the Lemma by these arguments. On the one hand, because the end a is regular, there exist n functions $w_k \in D_*$, $k = 1, ..., n$, vanishing near the singular end b and linearly independent modulo D_f, where D_f is the domain of the closure $\hat{f}$ of $\hat{f}^{(0)}$, $\hat{f} = \overline{\hat{f}^{(0)}}$. On the other hand, because the deficiency indices of $\hat{f}^{(0)}$, and therefore of $\hat{f}$ are equal to $n/2$, we have $\dim_{D_f} D_* = n$, whence it follows that any function $\psi_* \in D_*$ can be represented as $\psi_* = \psi + \sum_{k=1}^{n} c_k w_k$, where $\psi \in D_f$ and c_k are some number coefficients. The boundary value $[\chi_*, \psi_*](b)$ with any $\chi_*, \psi_* \in D_*$ is then represented as

$$[\chi_*, \psi_*](b) = [\chi_*, \psi](b) + \sum_{k=1}^{n} c_k [\chi_*, w_k](b)\ .$$

But the first term in the last equality vanishes by Lemma 9, see the second equality in (111) with the change $\psi_* \to \chi_*$, and the second term also vanishes because all w_k vanish near the singular end b, which proves the Lemma.

According to this Lemma, the term $[e_{U,k}, \psi_U](b)$ in boundary conditions (121) in Theorem 11 vanishes, and they reduces to $[e_{U,k}, \psi_U](a)$. Because the end a is regular, these s.a. boundary conditions are explicit in terms of boundary values of functions and their quasiderivatives at the end a,

$$\sum_{l,m=1}^{n} e_{U,k}^{[l-1]}(a)\,\mathcal{E}_{lm}\psi^{[m-1]}(a) = 0\,,\ k = 1, ..., n/2\,, \tag{135}$$

where $\mathcal{E}_{lm}$ are given by (124). If we introduce the rectangular $n \times n/2$ matrix

$$E_{1/2,U}(a) = \left|\left|E_{1/2,U,lk}(a)\right|\right|\ ,\ E_{1/2,U,lk}(a) = e_{U,k}^{[l-1]}(a)\ ,\ l = 1, ..., n\,,\ k = 1, ..., n/2\,, \tag{136}$$

s.a. boundary conditions (135) are written in the condensed form as $E_{1/2,U}^+(a)\,\mathcal{E}\Psi(a) = 0$. It seems useful to give a separate version of Theorem 11 for this case in the condensed notation.

Theorem 14 *Any s.a. operator $\hat{f}_U$ associated with an even s.a. differential expression $\check{f}$ of order n on an interval (a,b) with the regular and a and the singular end b in the case where the initial symmetric operator $\hat{f}^{(0)}$ has the deficiency indices $m_+ = m_- = n/2$, $U \in U(n/2)$, is given by*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{\psi_{f_U} \in D_* : E_{1/2,U}^+(a)\,\mathcal{E}\Psi_U(a) = 0\right\}\,, \\ \hat{f}_U \psi_U = \check{f}\psi_U\,, \end{cases} \tag{137}$$

where the matrix $\mathcal{E}$ is given by (124), the matrix $E_{1/2,U}(a)$ is given by (136), and $\Psi_U(a)$ is given by (126).

If the end a is singular while the end b is regular, a in (137) is changed to b.

The modified version of the two remarks to Theorem 11 in this case is

1) s.a. boundary conditions (137) are linearly independent, which is equivalent to the property that the rectangular $n \times n/2$ matrix $E_{1/2,U}(a)$ is of maximum rank,

$$\operatorname{rank} E_{1/2,U}(a) = \frac{n}{2}\,, \tag{138}$$

an analogue of (128);

2) relation (122) is written as

$$E^{+}_{1/2,U}(a)\,\mathcal{E} E_{1/2,U}(a) = 0 \tag{139}$$

which is an analogue of (129).

Of course, in applications, the condensed notation must be decoded.

As an illustration of Theorem 14, we consider the example of the deferential expression $\check{H}_0$ (94) on the semiaxis $[0,\infty)$. As to the deferential expression $\check{p}$ (38), we know from the previous section that there are no s.a. operators associated with $\check{p}$ on the semiaxis. The domain D_* in this case is the natural domain D_{0*} for $\check{H}_0$, it is given by (95) with the only change $\mathbb{R}^1 \to \mathbb{R}^1_+ = [0,\infty)$. The deficient subspaces $D_\pm$ as square-integrable solutions of eqs. (100),

$-\psi''_\pm = \pm i\kappa\psi_\pm$, are easily evaluated. It is sufficient to find D_+, then D_- is obtained by complex conjugation. Among the two linearly independent solutions

$$\psi_{+1,2} = \exp\left[\pm(1-i)\sqrt{\frac{\kappa}{2}}x\right]$$

of the equation for D_+, only one, $\exp\left[(i-1)\sqrt{\frac{\kappa}{2}}x\right]$, is square integrable on $[0,\infty)$. This means that the deficiency indices (m_+, m_-) in our case are $(1,1)$, and we have a one-parameter $U(1)$-family $\left\{\hat{H}_{0U}\right\}$, $U \in U(1)$, of s.a. operators in $L^2(0,\infty)$ associated with the differential expression $\check{H}_0$. Their specification by s.a. boundary conditions is performed in direct accordance with Theorem 14. The orthobasis vectors in $D_\pm$ are

$$e_\pm = \sqrt[4]{2\kappa}\exp\left[(\pm i - 1)\sqrt{\frac{\kappa}{2}}x\right]\,.$$

The group $U(1)$ is a circle and is naturally parametrized by an angle θ: $U = e^{i\theta}$, $-\pi \le \theta \le \pi$, $-\pi \backsim \pi$, therefore, $\hat{H}_{0U} = \hat{H}_{0\theta}$, and the single basis vector $e_U = e_\theta$ is

$$e_\theta = \sqrt[4]{2\kappa}\left\{\exp\left[(i-1)\sqrt{\frac{\kappa}{2}}x\right] + e^{i\theta}\exp\left[-(1+i)\sqrt{\frac{\kappa}{2}}x\right]\right\}\,.$$

The matrix $E_{1/2,U}(a)$ in (137) in our case is a 2×1 matrix, i.e., a column

$$E_{1/2,\theta}(0) = \sqrt[4]{2\kappa}\begin{pmatrix} 1 + e^{i\theta} \\ \sqrt{\frac{\kappa}{2}}\left[(i-1) - (1+i)\,e^{i\theta}\right]\end{pmatrix}$$

therefore, s.a. boundary conditions (137) become

$$\left(1+e^{-i\theta}\right)\psi_{\theta}'(0)-\sqrt{\frac{\kappa}{2}}\left[-(1+i)-(1-i)\,e^{i\theta}\right]\psi_{\theta}(0)=0\,,$$

or $\psi_{\theta}'(0)=\lambda\psi_{\theta}(0)$, where $\lambda=\lambda(\theta)$ is a ψ-independent dimensional parameter of dimension of inverse length

$$\lambda=\frac{\kappa}{2}\left(\tan\frac{\vartheta}{2}-1\right).$$

When θ ranges from $-\pi$ to π, λ ranges from $-\infty$ to $+\infty$, and $\lambda=\pm\infty$ $(\theta=\pm\pi)$ equivalently describe the s.a. boundary condition $\psi(0)=0$. It is natural to introduce the notation $\hat{H}_{0\lambda}=\hat{H}_{0\theta}$ and $\psi_{\lambda}=\psi_{\theta}$, with this notation, we finally obtain that any s.a. operator $\hat{H}_{0\lambda}$ associated with s.a. expression $\check{H}_0$ on the semiaxis $[0,\infty)$ is given by

$$\hat{H}_{0\lambda}:\left\{\begin{array}{l}D_{H_{0\lambda}}=\{\psi_{\lambda}:\psi_{\lambda},\,\psi_{\lambda}'\text{ a.c. on }[0,\infty)\,;\;\psi_{\lambda},\,\psi_{\lambda}''\in L^{2}(0,\infty)\,,\\ \psi'(0)=\lambda\psi(0)\,,\;-\infty\leq\lambda\leq\infty\}\,,\\ \hat{H}_{0\lambda}\psi_{\lambda}=-\psi_{\lambda}''\,.\end{array}\right. \tag{140}$$

Both $\lambda=\pm\infty$ yield the same boundary condition $\psi(0)=0$.

Each of these $\hat{H}_{0\lambda}$ is a candidate to the quantum-mechanical Hamiltonian for a free particle on a semiaxis. The boundary condition $\psi(0)=0$ is conventional in physics, but the boundary conditions $\psi'(0)=\lambda\psi(0)$ with a finite λ are also encountered. We note that a specific choice of the dimensional parameter κ appeared irrelevant as well as the normalization factor $\sqrt{\frac{\kappa}{2}}$, but if $\lambda\neq\pm\infty$, the dimensional parameter λ absent in $\check{H}_0$ enters the quantum theory as an additional specifying parameter.

By the way, the correctness of calculation which is rather simple in this case is confirmed by verifying that necessary conditions (138) and (139), $E_{1/2,\theta}^{+}(0)\,\mathcal{E}E_{1/2,\theta}(0)=0$, hold.

After the example, we return to the general questions. The specification of the s.a. differential operators $\hat{f}_U$ in terms of s.a. boundary conditions according to Theorems 11,12, and 14 requires evaluating the orthobasis functions $\{e_{+,k}\}_1^m$ and $\{e_{-,k}\}_1^m$ in the respective deficient subspaces D_+ and D_- , but only their boundary behavior is essential. In addition, there is an arbitrariness in the choice of the orthobasis functions, and the last example demonstrates that their specific boundary values do not actually enter the answer. All this allows suggesting that many analytical details are irrelevant from the standpoint of the general specification. And indeed, there is another way of specifying s.a. boundary conditions where the analytic task is replaced by some algebraic task avoiding the evaluation of the deficient subspaces provided that the deficient indices are known and equal, $m_+=m_-=m>0$. This way can be more convenient from the application standpoint. It is based on a modified version of the main theorem in the part related to formulas (35), (37). We therefore return to the main theorem and to the notation in the previous section, in particular, in (37), where an initial symmetric operator, its adjoint, and its closure are respectively denoted by $\hat{f}$, $\hat{f}^{+}$, and $\overline{\hat{f}}$and the vectors in their domains and in the domain D_{f_U} are denoted by ξ with appropriate subscripts.

We first note the evident fact that the vectors $e_{U,k}=e_{+,k}+\sum_{l=1}^{m}U_{lk}e_{-,l}$ in (37), forming a basis in the subspace $\left(D_{+}+\hat{U}D_{+}\right)\subset D_{f^{+}}$ of dimension m are linearly independent modulo $D_{\bar{f}}$. It is also evident that because all $e_{U,k}$ belong to D_{f_U} , the relation

$$\omega_{*}(e_{U,k},e_{U,l})=0\,,\;k,l=1,\ldots,m\,, \tag{141}$$

holds; in the case of s.a. differential operators, it becomes the already known relation (122). It appears that the really essential points are the linear independence of the m vectors $\{e_{U,k}\}_1^m$, modulo D_f and relation (141) for them.

We then note that the vectors $e_{U,k}$ in (37) can be equivalently replaced by their nondegenerate linear combinations, $e_{U,k} \to w_{U,k} = \sum_{a=1}^m X_{ak} e_{U,a}$, provided the matrix $X = \|X_{ak}\|$, $a, k = 1, \ldots, m$, is nonsingular, $\det X \neq 0$. As $e_{U,k}$, the vectors $w_{U,k}$ form a basis in the subspace $\left(D_+ + \hat{U} D_+\right)$ and are linearly independent modulo $D_{\bar{f}}$. Of course, relation (141) is extended to $\{w_{U,k}\}_1^m$ as the relation $\omega_* \left(w_{U,k}, w_{U,l}\right) = 0$. What is more, we can add arbitrary vectors $\underline{\xi}_k$ belonging to the domain $D_{\bar{f}}$ of the closure $\bar{f}$ to any vector $w_{U,k}$,

$$w_{U,k} \to w_k = w_{U,k} + \underline{\xi}_k = \sum_{a=1}^m X_{ak} e_{U,k} + \underline{\xi}_k\,, \ \underline{\xi}_k \in D_{\bar{f}}\,, \ k = 1, \ldots, m\,,$$

and obtain the equivalent description of the domain D_{f_U} of the s.a. extension $\hat{f}_U$ in terms of the m new vectors w_k,

$$D_{f_U} = \left\{\psi_U \in D_{f^+} : \omega_* \left(w_k, \psi_U\right) = 0\,, \ k = 1, \ldots, m\right\}\,, \qquad (142)$$

because $\omega_* \left(\underline{\xi}_k, \psi_U\right) = 0$ by (11), see also (13). By the same reason, relation (141) is also extended to the set $\{w_k\}_1^m$,

$$\omega_* \left(w_k, w_l\right) = 0\,, \ k, l = 1, \ldots, m\,. \qquad (143)$$

It is also evident that the m new vectors w_k are linearly independent modulo $D_{\bar{f}}$.

It appears that the converse is true. Let $\hat{f}$ be a symmetric operator with the adjoint $\hat{f}^+$ and the closure $\overline{\hat{f}}$, and let its deficiency indices be nonzero and equal, $m_+ = m_- = m > 0$, such that $D_f \subseteq D_{\bar{f}} \subset D_{f^+}$ and $\dim_{D_{\bar{f}}} D_{f^+} = 2m$. Let $\{w_k\}_1^m$ be a set of vectors with the following properties:

1) $w_k \in D_{f^+}\,, \ k = 1, \ldots, m\,;$

2) they are linearly independent modulo $D_{\bar{f}}$, i.e.,

$$\sum_{k=1}^m c_k w_k \in D_{\bar{f}}\,, \ \forall c_k \in \mathbb{C} \Longrightarrow c_k = 0\,, \ k = 1, \ldots, m\,;$$

3) relation (143), $\omega_* \left(w_k, w_l\right) = 0\,, \ k, l = 1, \ldots, m\,,$ holds for vectors w_k.

We then assert that the set $\{w_k\}_1^m$ defines some s.a. extension $\hat{f}_U$ of $\hat{f}$ as a s.a. restriction of the adjoint $\hat{f}^+$, $\hat{f} \subset \hat{f}_U = \hat{f}_U^+ \subset \hat{f}^+$ to the domain $D_{f_U} \subset D_{f^+}$ given by (142).

To prove this assertion, it is sufficient to prove that all the vectors w_k can be uniquely represented as

$$w_k = X_{ak} \left(e_{+,a} + \sum_{a=1}^m U_{ba} e_{-,b}\right) + \underline{\xi}_k\,,$$

where $\{e_{+,k}\}_1^m$ and $\{e_{-,k}\}_1^m$ are some orthobasises in the respective deficient subspaces D_+ and D_- of the symmetric operator $\hat{f}$, X_{ak} and U_{ba} are some coefficients such that the matrix X is nonsingular, and the matrix U is unitary, and the vectors $\underline{\xi}_k$ belong to $D_{\bar{f}}$, $\underline{\xi}_k \in D_{\bar{f}}$, $k = 1, \ldots, m$.

We first address to the condition 1). According to first von Neumann formula (5), any vector $w_k \in D_{f^+}$ is uniquely represented as

$$w_k = \xi_{+,k} + \xi_{-,k} + \underline{\xi}_k = \sum_{a=1}^{m} X_{ak} e_{+,a} + \sum_{a=1}^{m} Y_{ak} e_{-,a} + \underline{\xi}_k \, ,$$

where $\xi_{+,k} \in D_+$, $\xi_{-,k} \in D_-$, and $\underline{\xi}_k \in D_{\bar{f}}$, while X_{ak} and Y_{ak} , $a, k = 1, ..., m$, are the expansion coefficients of $\xi_{+,k}$ and $\xi_{-,k}$ with respect to the respective orthobasises $\{e_{+,k}\}_1^m$ and $\{e_{-,k}\}_1^m$. We now address to the conditions 2) and 3). The crucial remark is that these conditions imply that the matrices X and Y are nonsingular. The proof of that is by contradiction. Let, for example, the rank of X is nonmaximal, $\mathrm{rank}X < m$, this means that there exist a set $\{c_k\}_1^m$ of nontrivial complex constants c_k such that at least one of them is nonzero, but $\sum_{k=1}^{m} X_{ak} c_k = 0$, $a = 1, ..., m$. We thus have

$$\sum_{k=1}^{m} c_k \xi_{+,k} = \sum_{a=1}^{m} \left(\sum_{k=1}^{m} X_{ak} c_k \right) e_{+,a} = 0$$

and the vector $w = \sum_{k=1}^{m} c_k w_k$ is represented as

$$w = \xi_- + \underline{\xi} \, , \; \xi_- = \sum_{k=1}^{m} c_k \xi_{-,k} \, , \; \underline{\xi} = \sum_{k=1}^{m} c_k \underline{\xi}_k \, .$$

On the other hand, it follows from the condition 3) that

$$\omega_* (w, w) = \Delta_* (w) = \sum_{k,l=1}^{m} \bar{c}_k c_l \omega_* (w_k, w_l) = 0 \, .$$

By von Neumann formula (19), we then have $\Delta_* (w) = -2i\kappa \left|\left|\xi_-\right|\right|^2 = 0$, or $\xi_- = 0$, whence it follows that $w = \underline{\xi} \in D_{\bar{f}}$. But by the condition 2), the latter implies that all coefficients c_k are zero, which is a contradiction.

The proof of the nonsingularity of the matrix Y is similar.

The nonsingularity of the matrix X allows representing the vectors w_k as

$$w_k = \sum_{a=1}^{m} X_{ak} \left(e_{+,a} + \sum_{b=1}^{m} U_{ba} e_{-,b} \right) + \underline{\xi}_k \, ,$$

where the nonsingular matrix U is given by $U = YX^{-1}$, or $Y = UX$. Again appealing to condition 3) and to formula (18), we find

$$\omega_* (w_k, w_l) = \omega_* \left(\xi_{+,k} + \xi_{-,k} + \underline{\xi}_k \, , \xi_{+,l} + \xi_{-,l} + \underline{\xi}_l \right) = 2i\kappa \left[\left(\xi_{+,k}, \xi_{+,l} \right) - \left(\xi_{-,k}, \xi_{-,l} \right) \right] = 0 \, ,$$

or

$$\sum_{a,b=1}^{m} \left[\overline{X}_{ak} \left(e_{+,a}, e_{+,b} \right) X_{bl} - \overline{Y}_{ak} \left(e_{-,a}, e_{-,b} \right) Y_{bl} \right] = \sum_{a,b=1}^{m} \left[\overline{X}_{ak} X_{al} - \overline{Y}_{ak} Y_{al} \right] = 0 \, ,$$

$k,l=1,...,m$, where we use the condition that the sets $\{e_{+,k}\}_1^m$ and $\{e_{-,k}\}_1^m$ are orthonormalized, $(e_{+,a},e_{+,b})=(e_{-,a},e_{-,b})=\delta_{ab}$, $a,b=1,...,m$. The last equality can be written in the matrix form as

$$X^+X-Y^+Y=X^+\left[I-\left(\left(X^+\right)^{-1}Y^+\right)\left(YX^{-1}\right)\right]X=X^+\left(I-U^+U\right)X=0\,.$$

Because X is nonsingular, it follows that $U^+U=I$, i.e., the matrix U is unitary.

It is also seen how the unitary matrix U is uniquely restored from the given set of vectors $\{w_k\}_1^m$ under a certain choice of the orthobasises $\{e_{+,k}\}_1^m$ and $\{e_{-,k}\}_1^m$ in the respective deficient subspaces D_+ and D_- of the initial symmetric operator $\hat{f}$, which accomplish the proof of the above assertion.

We formulate the results of the above consideration as an addition to the main theorem which is a modification of the main theorem in the part related to formulas (35), (37).

Theorem 15 *(Addition to the main theorem.)*

Any s.a. extension $\hat{f}_U$ *of a symmetric operator* $\hat{f}$ *with the deficiency indices* $m_+=m_-=m>0$, $\hat{f}\subseteq\overline{\hat{f}}\subset\hat{f}_U=\hat{f}_U^+\subset\hat{f}^+$, *can be defined as*

$$\hat{f}_U:\left\{\begin{array}{l}D_{f_U}=\{\psi_U\in D_{f^+}:\,\omega_*(w_k,\psi_U)=0\,,\;k=1,...,m\}\,,\\ \hat{f}_U\psi_U=\hat{f}^+\psi_U\,,\end{array}\right. \tag{144}$$

where $\{w_k\}_1^m$ *is some set of vectors in* D_{f^+}, $w_k\in D_{f^+}$, $k=1,...,m$, *linearly independent modulo* $D_{\bar{f}}$ *and satisfying relation (143),* $\omega_*(w_k,w_l)=0$, $k,l=1,...,m$.

Conversely, any set $\{w_k\}_1^m$ *of vectors in* D_{f^+}, *linearly independent modulo* $D_{\bar{f}}$ *and satisfying relation (143) defines some s.a. extension of the symmetric operator* $\hat{f}$ *by (144).*

To be true, the $U(m)$ nature of the set $\left\{\hat{f}_U\right\}$ of all s.a. extensions is disguised in this formulation. This manifests itself in the fact that two sets $\{w_k\}_1^m$ and $\{\tilde{w}_k\}_1^m$ of vectors related by a nondegenerate linear transformation $\tilde{w}_k=\sum_{l=1}^m Z_{lk}w_l$, where the matrix $Z=||Z_{lk}||$ is nonsingular, defines the same s.a. extension. We can say that the description of s.a. extensions according to the addition to the main theorem is a description with some "excess", irrelevant, but controllable.

When applied to differential operators in $L^2(a,b)$, the addition to the main theorem yields an evident modification of Theorem 11. Formulating this modification, we return to the notation adopted in this section and omit the explanation of the conventional symbols.

Theorem 16 *Any s.a. operator* $\hat{f}_U$ *in* $L^2(a,b)$ *associated with a given s.a. differential expression* $\check{f}$ *in the case where the initial symmetric operator* $\hat{f}^{(0)}$ *with the closure* $\hat{f}$ *has the nonzero equal deficiency indices* $m_+=m_-=m$ *can be defined as*

$$\hat{f}_U:\left\{\begin{array}{l}D_{f_U}=\left\{\psi_U\in D_*:\;[w_k,\psi_U]|_a^b=0\,,\;k=1,...,m\right\},\\ \hat{f}_U\psi_U=\check{f}\psi_U\,,\end{array}\right. \tag{145}$$

where $\{w_k\}_1^m$ *is the set of functions belonging to* D_*, $w_k\in D_*$, $k=1,...,m$, *linearly independent modulo* D_f *and satisfying the relations*

$$[w_k,w_l]|_a^b=0\,,\;k,l=1,...,m. \tag{146}$$

Conversely, any set $\{w_k\}_1^m$ of functions belonging to D_*, linearly independent modulo D_f and satisfying relations (146) defines some s.a. operator associated with differential expression $\check{f}$ by (145).

The remark following the addition to the main theorem is completely applicable to Theorem 16.

Theorem 16 yields a modified version of Theorem 12 for the case of an even differential expression with the both regular ends where the deficiency indices are maximum. The modification consists in the replacement of the matrices $E_U(a)$ and $E_U(b)$ (125) of the boundary values of the basis functions $e_{U,k}$ and their quasiderivatives of order up to $n-1$ by the similar matrices

$$W(a) = \left|\left|W_{lk}(a) = w_k^{[l-1]}(a)\right|\right| \,,\; W(b) = \left|\left|W_{lk}(b) = w_k^{[l-1]}(b)\right|\right| \,,$$

generated by the functions $w_k \in D_*$ satisfying the conditions of Theorem 16. We assert that these conditions, the linear independence of the functions w_k modulo D_f and relation (146), are equivalent to the two respective conditions on the matrices $W(a)$ and $W(b)$:

1) the rank of a rectangular $2n \times n$ matrix $\mathbb{W}$ is maximum and equal to n,

$$\mathbb{W} = \begin{pmatrix} W(a) \\ W(b) \end{pmatrix},\; \mathrm{rank}\mathbb{W} = n, \tag{147}$$

this property is a complete analogue of (139);

2) the relation

$$W^+(b)\,\mathcal{E}W(b) = W^+(a)\,\mathcal{E}W(a) \tag{148}$$

holds.

The necessity of condition (147) is proved by contradiction. Let $\mathrm{rank}\mathbb{W} < n$. This means that there exists a set $\{c_k\}_1^n$ of nontrivial numbers, i.e., at least one of c_k is nonzero, such that

$$\sum_{k=1}^n W_{lk}(a)\,c_k = \sum_{k=1}^n w_k^{[l-1]}(a)\,c_k = 0\,,\; \sum_{k=1}^n W_{lk}(b)\,c_k = \sum_{k=1}^n w_k^{[l-1]}(b)\,c_k = 0\,.$$

By Lemma 9, this implies that the function $w = \sum_{k=1}^n c_k w_k$ belongs to D_f, the domain of the closure $\hat{f}$ of the initial symmetric operator $\hat{f}^{(0)}$, but because the functions w_k are linearly independent modulo D_f, this in turn implies that all c_k are zero which is a contradiction. We actually repeat the arguments leading to (139).

Conversely, let $W(a) = ||W_{lk}(a)||$ and $W(b) = ||W_{lk}(b)||$ be arbitrary matrices satisfying condition (147). Because the functions in D_* together with their quasiderivatives of order up to $n-1$ can take arbitrary values at the regular ends a and b, there exist a set $\{w_k\}_1^n$ of functions $w_k \in D_*$ such that

$$W_{lk}(a) = w_k^{[l-1]}(a)\;,\; W_{lk}(b) = w_k^{[l-1]}(b)\;,\; l,k = 1,...,n\,;$$

the functions w_k are evidently linearly independent modulo D_f.

As to relation (148), this relation is equivalent to relation (146) in view of formulas (88), (89) where χ_* and ψ_* are replaced by the respective w_k and w_l , $l,k = 1,...,n$, and formula (73); it is the copy and extension of relation (129). Because the functions w_k are represented in

this context only by the boundary values of their quasiderivatives of order from 0 up to $n-1$, it is natural to introduce the notation

$$A = ||a_{lk}|| = W(a) \ , \ B = ||b_{lk}|| = W(b)$$

and formulate a modification of Theorem 16 as follows:

Theorem 17 *Any s.a. operator $\hat{f}_U$ in $L^2(a,b)$ associated with an even s.a. differential expression $\check{f}$ of order n with both regular ends can be defined as*

$$\hat{f}_U : \begin{cases} D_{f_U} = \{\psi_U \in D_* : \ B^+ \mathcal{E} \Psi_U(b) = A^+ \mathcal{E} \Psi_U(a)\} \ , \\ \hat{f}_U \psi_U = \check{f} \psi_U \ , \end{cases} \tag{149}$$

where A and B are some $n \times n$ matrices satisfying the conditions

$$\operatorname{rank} \begin{pmatrix} A \\ B \end{pmatrix} = n \, , \ B^+ \mathcal{E} B = A^+ \mathcal{E} A \, , \tag{150}$$

the matrix $\mathcal{E}$ and the columns $\Psi_U(b)$ and $\Psi_U(a)$ are respectively given by (124), and (126).

Conversely, any two matrices A and B satisfying conditions (150) define some s.a. operator associated with the s.a. differential expression $\check{f}$ by (149).

Again, as after Lemma 8 and after Theorem 12, we can add that a similar theorem holds for any s.a. differential expression $\check{f}$ of any order with differentiable coefficients and the both regular ends with the change quasiderivatives to usual derivatives if boundary values (89) are finite forms in the boundary values of functions and their derivatives.

The remarks after the addition to the main theorem 15 and Theorem 16 on the hidden $U(n)$-nature of n s.a. boundary conditions (149) become the remark that the matrices $\tilde{A} = AZ$ and $\tilde{B} = BZ$, where the matrix $Z = ||z_{lk}||$, $l,k = 1,...,n$, is nonsingular, define the same s.a. operator.

Actually, this arbitrariness in the choice of the matrices A and B is unremovable only if their ranks are not maximum[54], $\operatorname{rank} A < n$, $\operatorname{rank} B < n$, i.e., if they are singular, $\det A = \det B = 0$ (we note that condition (150) implies that the matrices A and B are singular or nonsingular simultaneously). If these matrices are nonsingular, which is a general case, the arbitrariness can be eliminated. Really, let $\det B \neq 0$, therefore, $\det A \neq 0$ also. Then, with taking the property $\mathcal{E}^{-1} = -\mathcal{E}$ of the nonsingular matrix $\mathcal{E}$ into account, s.a. boundary conditions (149) can be represented as

$$\Psi(b) = S\Psi(a) \ , \text{ or } \Psi(a) = S^{-1}\Psi(b) \ , \tag{151}$$

where the nonsingular matrix S is $S = -\mathcal{E}\left(AB^{-1}\right)^+ \mathcal{E}$. Because the matrix $\mathcal{E}$ is anti-Hermitian, $\mathcal{E}^+ = -\mathcal{E}$, the adjoint S^+ is $S^+ = -\mathcal{E}\left(AB\right)^{-1} \mathcal{E}$ and the second condition in (150) is represented in terms of S as

$$S^+ \mathcal{E} S = \mathcal{E} \, , \tag{152}$$

otherwise, S is arbitrary.

The algebraic sense of relation (152) is clear: it means that the linear transformations

$$\Psi \to S\Psi \tag{153}$$

[54] Of course, this condition is compatible with condition (150).

defined in the n-dimensional linear space of n-columns Ψ with elements $\psi_i\,,\ i=1,...,n$, preserve the Hermitian sesquilinear form $\chi^{+}\left(\frac{1}{i}\mathcal{E}\right)\Psi$, or equivalently, the Hermitian quadratic form $\Psi^{+}\left(\frac{1}{i}\mathcal{E}\right)\Psi$. The Hermitian matrix $\frac{1}{i}\mathcal{E}$ can be easily diagonalized by a unitary transformation,

$$\frac{1}{i}\mathcal{E}=T^{+}\Sigma T\,, \tag{154}$$

where the diagonal $n\times n$ matrix Σ is

$$\Sigma=\operatorname{diag}\left(I,-I\right)\,, \tag{155}$$

I is the $n/2\times n/2$ unit matrix, and the unitary matrix $T=||T_{lm}||\,,\ l,m=1,...,n\,,\ T^{+}T=\mathbf{I}\,$, is

$$\begin{gathered}T_{lm}=\frac{1}{\sqrt{2}}\left\{\delta_{l,m}\left[\theta\left(\frac{n+1}{2}-m\right)-i\theta\left(m-\frac{n+1}{2}\right)\right]\right.\\ \left.\delta_{l,n+1-m}\left[\theta\left(\frac{n+1}{2}-m\right)+i\theta\left(m-\frac{n+1}{2}\right)\right]\right\}\,,\end{gathered} \tag{156}$$

and $\theta\left(x\right)$ is the well-known step function,

$$\theta\left(x\right)=\left\{\begin{array}{l}1\,,\ x>0\\ 0\,,\ x<0\end{array}\right.\,,$$

and we see that the signature of the matrix $\frac{1}{i}\mathcal{E}$ is $\left(\frac{n}{2},\frac{n}{2}\right)$, which implies that the transformations S given by (153) and satisfying (152) form the group $U\left(\frac{n}{2},\frac{n}{2}\right)$. We thus find that some of s.a. boundary conditions, to be true, the most of them, are parametrized by elements of the group $U\left(\frac{n}{2},\frac{n}{2}\right)$, which defines an embedding of the group $U\left(\frac{n}{2},\frac{n}{2}\right)$ into the group $U\left(n\right)$ parameterizing all the s.a. boundary conditions. This embedding is an embedding "into", but not "onto": although $U\left(\frac{n}{2},\frac{n}{2}\right)$ is an n^2-parameter manifold as $U\left(n\right)$, the group $U\left(\frac{n}{2},\frac{n}{2}\right)$ is noncompact, whereas $U\left(n\right)$ is compact; it is also clear from the aforesaid that the s.a. boundary conditions (149) with the singular matrices A and B cannot be represented in form (151). Such boundary conditions can be obtained by some limit procedure where some matrix element of S tends to infinity while others vanish (we note that $|\det S|=1$). This procedure corresponds to a compactification of $U\left(\frac{n}{2},\frac{n}{2}\right)$ to $U\left(n\right)$ by adding some limit points.

We must note that looking at the representation of the sesquilinear asymmetry form ω_* in terms of boundary values of functions and their quasiderivatives in the case of an even s.a. differential expression with the both regular ends[55]

$$\omega_*\left(\chi_*,\psi_*\right)=\chi_*^{+}\left(b\right)\mathcal{E}\Psi_*\left(b\right)-\chi_*^{+}\left(a\right)\mathcal{E}\Psi_*\left(a\right)\,, \tag{157}$$

where the n-columns $\chi_*\left(a\right),\chi_*\left(b\right)$, and $\Psi_*\left(a\right),\Psi_*\left(b\right)$ are given by (126) with the respective changes $\psi_U\rightarrow\chi_*$ and $\psi_U\rightarrow\psi_*$, it is easy to see from the very beginning that boundary conditions (151) with any fixed matrix S satisfying (152) result in vanishing the asymmetry form ω_* and thus define a symmetric restriction of the adjoint $\hat{f}^*$. Using the standard technique of evaluating the adjoint in terms of ω_* (157), it is also easy to prove that boundary condition (151),

[55]This representation based on formulas (88), (89), (73), and (126) was actually used above in the consideration related to formulas (123)-(129).

(152) are actually s.a. boundary conditions defining a s.a. restriction of $\hat{f}^{*}$. Unfortunately, these are not all possible s.a. boundary conditions.

It seems instructive to illustrate Theorem 17 and also s.a. boundary conditions (151), (152) based on representation (157) for ω_{*} and their extensions to s.a. differential expressions of any order with the both regular ends by our examples of the s.a. differential expressions $\check{p}$ (38) and $\check{H}_0$ (94) on an interval $(0, l)$.

As to $\check{p}$, an analogue of (157) for $\hat{p}^{*}$ (39) is

$$\omega_{*}\left(\chi_{*}, \psi_{*}\right) = -i\left(\overline{\chi_{*}}\left(l\right)\psi\left(l\right) - \overline{\chi}\left(0\right)\psi\left(0\right)\right), \tag{158}$$

see (40)–(43). It immediately follows the s.a. boundary conditions

$$\psi_{\vartheta}\left(l\right) = e^{i\vartheta}\psi_{\vartheta}\left(0\right), \tag{159}$$

with arbitrary but fixed angle ϑ, $0 \leq \vartheta \leq 2\pi$, $0 \backsim 2\pi$, which coincides with boundary conditions (52) defining s.a. operators $\hat{p}_{\vartheta}$ (54). In this case, thus obtained boundary conditions (159) yield all the $U(1)$-family of s.a. operators associated with the s.a. deferential expression $\check{p}$ (38) on an interval $[0, l]$.

As to $\check{H}_0$, we show how the already known s.a. boundary conditions (130)–(133) are obtained without evaluating the deficient subspaces.

Let

$$A = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \; B = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

it is easy to verify that they satisfy conditions (150), then formula (149) yields the s.a. boundary conditions $\psi\left(0\right) = \psi\left(l\right) = 0$ coinciding with (131). These boundary conditions can be obtained from boundary conditions (151) with

$$S\left(\varepsilon\right) = \begin{pmatrix} 0 & \varepsilon \\ -1/\varepsilon & 0 \end{pmatrix}$$

in the limit $\varepsilon \rightarrow 0$, such $S\left(\varepsilon\right)$ arises if we slightly deform the initial A and B,

$$A{\rightarrow}A\left(\varepsilon\right) = \begin{pmatrix} \varepsilon & 0 \\ 0 & 1 \end{pmatrix}, \; B{\rightarrow}B\left(\varepsilon\right) = \begin{pmatrix} 0 & -\varepsilon \\ 1 & 0 \end{pmatrix},$$

removing their singularity without violating conditions (150).

Let now

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \; B = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

these matrices also satisfy (150), then formula (149) yields the s.a. boundary conditions $\psi'\left(0\right) = \psi'\left(l\right) = 0$ coinciding with (132). Again, these boundary conditions can be obtained from boundary conditions (151) with

$$S\left(\varepsilon\right) = \begin{pmatrix} 0 & -1/\varepsilon \\ \varepsilon & 0 \end{pmatrix}$$

in the limit $\varepsilon \rightarrow 0$, this $S\left(\varepsilon\right)$ arises as a result of a deformation

$$A \rightarrow A\left(\varepsilon\right) = \begin{pmatrix} 0 & 1 \\ -\varepsilon & 0 \end{pmatrix}, \; B \rightarrow B\left(\varepsilon\right) = \begin{pmatrix} 1 & 0 \\ 0 & \varepsilon \end{pmatrix}.$$

If we take

$$A=\begin{pmatrix} 0 & a_2 \\ 0 & a_4 \end{pmatrix} \; , \; B=\begin{pmatrix} b_1 & 0 \\ b_3 & 0 \end{pmatrix} \; ,$$

where at least one number in the pairs a_2, a_4 and b_1, b_3 is nonzero, which is required by the first condition in (150) and also $a_2\overline{a_4}=\overline{a_2}a_4$ and $b_1\overline{b_3}=\overline{b_1}b_3$, which is required by second condition in (150), we obtain the so called splitted boundary conditions

$$\psi'(0)=\lambda\psi(0) \; , \; \psi'(l)=\mu\psi(l) \; , \tag{160}$$

where λ and μ are arbitrary numbers, $-\infty\leq\lambda$, $\mu\leq+\infty$, $-\infty\backsim+\infty$, and the both $\lambda=\pm\infty$ yield $\psi(0)=0$ while $\mu=\pm\infty$ yield $\psi(l)=0$.

Taking $S=I$ in (151), we obtain the periodic boundary conditions

$$\psi(0)=\psi(l) \; , \; \psi'(0)=\psi'(l)$$

coinciding with (133). If we take $S=e^{i\vartheta}I$, $0\leq\vartheta\leq 2\pi$, $0\backsim 2\pi$, we obtain the modified periodic s.a. boundary conditions

$$\psi(l)=e^{i\vartheta}\psi(0) \; , \; \psi'(l)=e^{i\vartheta}\psi'(0) \tag{161}$$

including periodic, $\vartheta=0$, and antiperiodic, $\vartheta=\pi$, boundary conditions. It is interesting to note that these s.a. boundary conditions define the s.a. operator $\hat{H}_{0\vartheta}$ which can also be represented as

$$\hat{H}_{0\vartheta}=\hat{p}_{\vartheta}^2 \, . \tag{162}$$

The one-parameter family $\{H_{0\vartheta}\}$ of s.a. operators (162) among the whole four-parameter family of s.a. operators associated with the s.a. differential expression $\check{H}_0$ immediately follows from the Akhiezer-Glazman theorem (Theorem 4) with $\hat{a}=\hat{a}^+=\hat{p}_\vartheta$, after constructing s.a. operator $\hat{p}_\vartheta$ (54).

As to the "entangled" s.a. boundary conditions (130), it is easy to verify that they can be represented in form (151), $\Psi(l)=S\Psi(0),$, where the matrix

$$S=-\begin{pmatrix} \cosh\pi & \frac{l}{\pi}\sinh\pi \\ \frac{\pi}{l}\sinh\pi & \cosh\pi \end{pmatrix}$$

satisfies condition (152).

Our concluding remark is that the s.a. operators associated with s.a. differential expressions $\check{H}$ (65) with $V=\overline{V}$, conventionally attributed to the quantum-mechanical energy a particle on an interval $[0,l]$ in a potential field V, are specified by the same boundary conditions if V is integrable on $[0,l]$ because under this conditions, the ends of the interval remain regular. It is completely clear in the case of a bounded potential, $|V(x)|<M$, because the addition of a bounded s.a. operator defined everywhere to a s.a. operator with a certain domain yields a s.a. operator with the same domain.

Theorem 16 yields also a modified version of Theorem 14. Because the appropriate consideration is completely similar to the previous one resulting in Theorem 17, we directly formulate this modification.

Theorem 18 *Any s.a. operator $\hat{f}_U$ associated with an even s.a. deferential expression $\check{f}$ of order n on an interval (a,b) with the regular end a and the singular end b in the case where*

the initial symmetric operator $\hat{f}^{(0)}$ has the minimum deficiency indices $m_+ = m_- = n/2$, $U \in U(n/2)$, can be defined as

$$
\hat{f}_U : \left\{ \begin{array}{l} D_{f_U} = \left\{ \psi_U(x) \in D_* : \ A^+_{1/2} \mathcal{E} \psi_U(a) = 0 \right\} , \\ \hat{f}_U \psi_U = \check{f} \psi_U , \end{array} \right. \tag{163}
$$

where $A_{1/2}$ is some rectangular $n \times n/2$ matrix satisfying the conditions

$$
\operatorname{rank} A_{1/2} = n/2 \tag{164}
$$

and

$$
A^+_{1/2} \mathcal{E} A_{1/2} = 0 \, , \tag{165}
$$

the matrix $\mathcal{E}$ and the column $\Psi_U(a)$ are respectively given by (124), and (126).

Conversely, any $n \times n/2$ matrix A satisfying (164) and (165) define some s.a. operator associated with the s.a. differential expression $\check{f}$ by (163).

If the end a is singular while the end b is regular, $A_{1/2}$ and a in (163)–(165) are replaced by the respective $B_{1/2}$ and b.

Similarly to Theorem 17, this theorem is accompanied by the remark on the hidden $U(n/2)$-nature of boundary conditions (163): the matrices $A_{1/2}$ and $A_{1/2}Z$, where Z is some nonsingular $n/2 \times n/2$ matrix, yield the same s.a. operator.

We illustrate this theorem by the example of the deferential expression $\check{H}$ (65) with $V = \overline{V}$, on the semiaxis $[0, \infty)$ (the quantum-mechanical energy of a particle on the semiaxis in the potential field V). We begin with the differential expression $\check{H}_0$ (94) (a free particle) already considered as an illustration after Theorem 14 where it was shown that the corresponding deficiency indices are $(1, 1)$ and show how the known result is obtained without evaluating the deficient subspaces, which allows extending the results to the case $V \neq 0$. In this case, $n = 2$, $n/2 = 1$, the matrix $A_{1/2}$ is a two column with elements a_1, a_2, where at least one of the numbers in the pair a_1, a_2 is nonzero, which is required by condition (164), while condition (165) requires $\overline{a_1} a_2 = a_1 \overline{a_2}$. Formula (163) then yields the already known s.a. boundary conditions

$$
\psi'(0) = \lambda \psi(0) \ , \ \lambda \in \mathbb{R}^1 \, , \tag{166}
$$

where $\lambda = \overline{a_2}/\overline{a_1} = a_2/a_1$ is an arbitrary, but fixed, real number, $-\infty \leq \lambda \leq \infty$, $-\infty \backsim \infty$; $\lambda = \pm\infty$ correspond to the boundary condition $\psi(0) = 0$. These boundary conditions defining s.a. operators $\hat{H}_{0\lambda}$ (140) are well known in physics.

It is evident that the same boundary conditions specify the s.a. operators $\hat{H}_\lambda$ associated with the s.a. differential expressions $\check{H}$ (65) in the case where the potential is bounded, $|V(x)| < M$, and $\hat{H}_\lambda$ is then defined on the some domain as $\hat{H}_{0\lambda}$.

We now shortly discuss the physically interesting question of under which conditions on the potential $V(x)$, the s.a. differential expression $\check{H}$ (65) on $[0, \infty)$ also falls under Theorem 18 as the differential expression $\check{H}_0$ (94), and is therefore specified by the same s.a. boundary conditions (166).

For the left end to remain regular, it is necessary that $V(x)$ be integrable at the origin, i.e., integrable on any segment $[0, a]$, $a < \infty$. We know that if the left end is regular, the deficiency indices of the associated symmetric operator $\hat{H}^{(0)}$ can be $(1, 1)$ or $(2, 2)$, and we

need criteria for these be minimum, but not maximum. At this point, we address to some useful general result on the maximum deficiency indices (n,n) for the symmetric operator $\hat{f}^{(0)}$ associated with an even s.a. differential expression $\check{f}$ of order n with one regular end and one singular end. It appears that the occurrence of the maximum deficiency indices is controlled by the dimension of the kernel of the adjoint $\hat{f}^{*}$, $\dim\ker f^{*}$, or by the number of the linearly independent square-integrable solutions of the homogeneous equation $\check{f}u=0$. Namely, $\hat{f}^{(0)}$ has maximum deficiency indices $m_{+}=m_{-}=n$ iff the homogeneous equation has the maximum number n of linearly independent square-integrable solutions, in other words, iff the whole fundamental system $\{u_i\}_1^n$ of solutions of the homogeneous equation lies in $L^2(a,b)$; the same is true for the homogeneous equation $\check{f}u=\lambda u$ with any real λ.

It follows from this general statement that in order to have the deficiency indices $(1,1)$ in our particular case where $n=2$, it is sufficient to point out the conditions on V under which the homogenous equation $-u''+Vu=0$ has at lest one non-square-integrable solution. A few of such conditions are known since Weyl [23]. We cite the two which seem rather general and also simple from the application standpoint and formulate them directly in the form relevant to the deficiency indices: the symmetric operator $\hat{H}^{(0)}$ has deficiency indices $(1,1)$ if

$$1)\; V(x)\in L^2(0,\infty)\,, \tag{167}$$

i.e., the potential V is square-integrable, [30], or

$$2)\; V(x)>-Kx^2\,,\; K>0\,, \tag{168}$$

for sufficiently large x [31]. Condition (168) is a particular case of a more general condition [32]. For the proofs, other conditions and details, see [8]. We here don't dwell on the proofs because we independently obtain the same results in another context later, but make several remarks concerning physical applications.

We consider it useful, in particular, for further references, to repeat once more that under conditions (167) or (168) on the potential V integrable at the origin, all s.a. Hamiltonians associated with the s.a. differential expression $\check{H}$ (65) on the semiaxis $[0,\infty)$ form a one-parameter family $\left\{\hat{H}_\lambda\right\}$, $-\infty\leq\lambda\leq\infty$, $-\infty\backsim\infty$, and any $\hat{H}_\lambda$ is specified by s.a. boundary conditions (166):

$$\hat{H}_\lambda:\left\{\begin{array}{l} D_\lambda=\{\{\psi_\lambda:\psi_\lambda,\psi_\lambda'\text{ a.c. on }[0,\infty)\,;\psi_\lambda,-\psi_\lambda''+V\psi_\lambda\in L^2(0,\infty)\,;\psi_\lambda'(0)=\lambda\psi_\lambda(0)\}\,,\\ \hat{H}_\lambda\psi_\lambda=-\psi_\lambda''+V\psi_\lambda\,.\end{array}\right. \tag{169}$$

Condition (167) covers the conditions of the regularity of the left end because it automatically implies that V is integrable at the origin. By the way, this conditions does not at all imply that V vanishes at infinity, the potential can have growing peaks of any sign with growing x.

The majority of potentials encountered in physics, in particular, the potentials vanishing or growing at infinity, satisfy condition (168). Criterion (168) is optimal in the sense that if $V\backsim -Kx^{2(1+\varepsilon)}$ as $x\to\infty$, where $\varepsilon>0$ can be arbitrarily small, the both linearly independent solutions $u_{1,2}$ of the homogenous equation $-u''+Vu=0$, and also of the equation $-u''+Vu=\lambda u$ with any real λ, are square integrable:

$$u_{1,2}(x)\backsim\frac{1}{x^{(1+\varepsilon)/2}}\exp\left[\pm i\frac{K^{1/2}}{2+\varepsilon}x^{2+\varepsilon}\right]\,,\; x\to\infty\,,$$

therefore, the deficiency indices of the symmetric operator $\hat{H}^{(0)}$ are $(2,2)$ and the s.a. boundary conditions include boundary conditions at ∞. This circumstance is crucial in the sense that its neglecting leads to some "paradox". From the naive standpoint, the situation where the stationary Schrödinger equation $-\psi'' + V\psi = E\psi$ has only square-integrable solutions for any real energy E, apparently implies that all the eigenstates in such a potential are bound, and what is more, the discrete energy spectrum turns out to be continuous, which is impossible. This situation is quite similar to the case of a "fall to the center" for a particle of negative energy in a strongly attractive potential[56] $V(x) < -\frac{1}{4x^2}$ as $x \to 0$. The resolution of the paradox is in the obligatory boundary conditions at infinity; without these boundary conditions, we actually deal with the Hamiltonian $\hat{H}^*$ that is non-s.a.. Only taking s.a. boundary conditions at infinity into account, we get a s.a. Hamiltonian all the eigenstates of which are bound, but the spectrum is really discrete.

We must also emphasize that the condition of the integrability of the potential V at the origin providing the regularity of the left end is also crucial. The case where the potential is singular and nonintegrable at the origin requires a special consideration.

The last remark concerns the Hamiltonian for a particle moving along the real axis in the potential field V. If $V(x)$ is a locally integrable function[57], the Hamiltonian is defined as a s.a. operator associated with the previous differential expression $\check{H}$ (65), but now on the whole real axis $\mathbb{R}^1 = (-\infty, +\infty)$ and with the both singular ends, $-\infty$ and $+\infty$. Let $\hat{H}^{(0)}$ be the initial symmetric operator associated with $\check{H}$. The crucial remark is that according to formula (107), its deficiency indices $m_+ = m_- = m$ are defined by the deficiency indices $m_+^{(-)} = m_-^{(-)} = m^{(-)}$ and $m_+^{(+)} = m_-^{(+)} = m^{(+)}$ of the respective symmetric operators $\hat{H}_-^{(0)}$ and $\hat{H}_+^{(0)}$ associated with the same differential expression $\check{H}$ restricted to the respective negative semiaxis $\mathbb{R}_-^1 = (-\infty, 0]$ and positive semiaxis $\mathbb{R}_+^1 = [0, +\infty)$:

$$m = m^{(-)} + m^{(+)} - 2\,. \tag{170}$$

Let the potential V satisfy one of the conditions that are the extensions of conditions (167) and (168) to the whole real axis $\mathbb{R}^1$,

$$1)\ V(x) \in L^2(-\infty, +\infty)\,, \tag{171}$$

i.e., V is square integrable on $\mathbb{R}^1$, or

$$2)\ V(x) > -Kx^2\,,\ K > 0\,, \tag{172}$$

for sufficiently large $|x|$. Then the symmetric operator $\hat{H}_+^{(0)}$ satisfies conditions (167) or (168), and therefore, its deficiency indices are $(1,1)$, i.e., $m^{(+)} = 1$; the same is evidently true for the symmetric operator $\hat{H}_-^{(0)}$, it is sufficient to change the variable $x \to -x$, i.e., $m^{(-)} = 1$ also. It follows by (170) that $m = 1 + 1 - 2 = 0$, i.e., the deficiency indices of the symmetric operator $\hat{H}^{(0)}$ are $(0,0)$. This means that $\hat{H}^{(0)}$ is essentially s.a., and its unique s.a. extension is $\hat{H} = \hat{H}^*$.

We note that the same result follows from a consideration of the asymmetry form ω_* for $\hat{H}^*$. According to (88) and (89), it is given by

$$\omega_*(\chi_*, \psi_*) = [\chi_*, \psi_*]|_{-\infty}^{\infty}\,,\ \forall \chi_*, \psi_* \in D_*\,, \tag{173}$$

[56] It can be respectively called a "fall to infinity" because a classical particle escapes to infinity in a finite time.

[57] That is, if $V(x)$ is integrable on any segment $[a, b]$, $-\infty < a < b < \infty$.

where $[\chi_*, \psi_*] = -\overline{\chi_*}\psi_*' + \overline{\chi_*'}\psi_*$. The crucial remark is then that the restrictions of the functions $\psi_* \in D_*$ to the respective semiaxis $\mathbb{R}_-^1$ and $\mathbb{R}_+^1$ evidently belong to the domains of the respective adjoints $\hat{H}_-^* = \left(\hat{H}_-^{(0)}\right)^+$ and $\hat{H}_+^* = \left(\hat{H}_+^{(0)}\right)^+$ and therefore $[\chi_*, \psi_*]$ have the same boundary values at infinity as the respective boundary values for $\hat{H}_-^*$ and $\hat{H}_+^*$. But if the deficiency indices of $\hat{H}_-^{(0)}$ and $\hat{H}_+^{(0)}$ are $(1,1)$, the corresponding boundary values are identically zero. It follows that ω_* (173) in this case is identically zero as well, and the adjoint $\hat{H}^*$ is symmetric, and therefore is s.a. We return to these arguments later where we independently prove the vanishing of the boundary values $[\chi_*, \psi_*](\infty)$ for $\hat{H}_+^{(0)}$.

The final conclusion is that under conditions (171) or (172), there is a unique s.a. operator $\hat{H}$ associated with a s.a. differential expression $\check{H}$ (65) on the real axis $\mathbb{R}^1$ and defined on the natural domain:

$$\hat{H}:\left\{\begin{array}{l} D_H = \left\{\psi(x) : \psi,\, \psi' \text{ a.c. in } \mathbb{R}^1;\ \psi,\, -\psi'' + V\psi \in L^2(-\infty, +\infty)\right\}, \\ \hat{H}\psi = -\psi'' + V\psi\,. \end{array}\right.$$

This fact is implicitly adopted in the majority of textbooks on quantum mechanics for physicists and considered an unquestionable common place. In particular, it concerns the one-dimensional Hamiltonians with bounded potentials like a potential barrier, a finite well, a solvable potentials like $V_0 \mathrm{ch}^{-2}(ax)$, the Hamiltonians with growing potentials, for example, the Hamiltonian for a harmonic oscillator where $\check{H} = -d^2/dx^2 + x^2$, and even the Hamiltonians with linear potential $V = kx$, which goes to $-\infty$ at one of the ends, but only linearly, not faster than quadratically.

As to the harmonic oscillator Hamiltonian, it follows from the Akhiezer–Glazman theorem (Theorem 4) that its standard representation $\hat{H} = \hat{a}^+\hat{a} + 1$ implies that $\hat{a}$ is the closed operator associated with the non-s.a. differential expression $\check{a} = d/dx + x$ and defined by

$$\hat{a}:\left\{\begin{array}{l} D_a = \left\{\psi(x) : \psi \text{ a.c. in } (-\infty, +\infty);\ \psi, (d/dx + x)\psi \in L^2(-\infty, +\infty)\right\}, \\ \hat{a}\psi = (d/dx + x)\psi\,, \end{array}\right.$$

while $\hat{a}^+$ is its adjoint, it is the operator associated with the non-s.a. differential expression $\check{a}^+ = -d/dx + x$ and defined by

$$\hat{a}^+:\left\{\begin{array}{l} D_{a^+} = \left\{\psi_*(x) : \psi_* \text{ a.c. in } (-\infty, +\infty);\ \psi_*, (-d/dx + x)\psi_* \in L^2(-\infty, +\infty)\right\}, \\ \hat{a}^+\psi_* = (-d/dx + x)\psi_*\,. \end{array}\right.$$

These subtle points are usually omitted in the physical literature. To be true, they are irrelevant for finding the eigenfunctions of $\hat{H}$ because the latter are smooth functions exponentially vanishing at infinity.

The other remarks on the physical applicability of conditions (167) and (168) are naturally and practically literally extended to conditions (171) and (172). In particular, if condition (172) is violated, and, for example, $V(x) < -Kx^{2(1+\varepsilon)}$, $\varepsilon > 0$, as $x \to -\infty$ or/and $x \to \infty$, we respectively have $m^{(-)} = 2$ or/and $m^{(+)} = 2$ and consequently $m = 1$ or $m = 2$. In this case, we have the respective one-parameter $U(1)$-family or four-parameter $U(2)$-family of s.a. Hamiltonians $\left\{\hat{H}_U\right\}$, $U \in U(1)$ or $U \in U(2)$, that are specified by some s.a. boundary conditions at infinity, $x = -\infty$ or/and $x = \infty$. To be true, such potentials are considered apparently nonphysical at present (unless they emerge in some exotic cosmological scenarios).

3.8 Alternative way of specifying self-adjoint differential operators in terms of explicit self-adjoint boundary conditions

The description of s.a. extensions of symmetric differential operators in terms of s.a. boundary conditions due to the above presented conventional methods is sometimes of an inexplicit character, especially for the case of singular ends, such that the $U(m)$ nature of the whole family of s.a. extensions is not evident.

We now discuss a possible alternative way of specifying s.a. differential operators associated with a given s.a. differential expression in terms of explicit, in general asymptotic, s.a. boundary conditions, the $U(m)$ nature of this specification is evident. The idea of the method is a result of two observations. The both equally concerns the asymmetry forms ω_* and Δ_*. For definiteness, we speak about the quadratic asymmetry form Δ_*, although the all to be said applies to ω_*: we recall that Δ_* and ω_* define each other.

For the first observation, we return to the previous section, but use the notation adopted in this section for differential operators where the elements of the Hilbert space $L^2(a,b)$ are denoted by ψ with an appropriate subscript, the closure of the initial symmetric operator $\hat{f}^{(0)}$ is denoted by $\hat{f}$, $\overline{\hat{f}^{(0)}} = \hat{f}$, the deficient subspaces are denoted by D_+ and D_- with $z = i\kappa$, and etc.

By first von Neumann formula (5), any $\psi_* \in D_*$ is uniquely represented as

$$\psi_* = \psi + \psi_+ + \psi_- \,,\ \psi \in D_f \,,\ \psi_+ \in D_+ \,,\ \psi_- \in D_- \,.$$

By von Neumann formula (19), the asymmetry form Δ_* is nontrivial only on the direct sum $D_+ + D_-$ of the deficient subspaces and expressed in terms of D_+ and D_- components of ψ_* as

$$\Delta_*(\psi_*) = 2i\kappa\left(\left|\left|\psi_+\right|\right|^2 - \left|\left|\psi_-\right|\right|^2\right) .$$

Let $\{e_{+,k}\}_1^{m_+}$ and $\{e_{-,k}\}_1^{m_-}$ be some orthobasises in the respective D_+ and D_- such that

$$\psi_+ = \sum_{k=1}^{m_+} c_{+,k} e_{+,k} \,,\ \psi_- = \sum_{k=1}^{m_-} c_{-,k} e_{-,k} \,,$$

where $c_{\pm,k}$ are the respective expansion coefficients, then the asymmetry form Δ_* becomes

$$\Delta_*(\psi_*) = 2i\kappa\left(\sum_{k=1}^{m_+} \left|c_{+,k}\right|^2 - \sum_{k=1}^{m_-} \left|c_{-,k}\right|^2\right) . \tag{174}$$

The problem of symmetric and s.a. extensions of the initial symmetric operator $\hat{f}^{(0)}$ can be considered in terms of the expansion coefficients. The deficient subspaces D_+ and D_- reveals itself as the respective complex linear spaces $\mathbb{C}_+^{m_+}$ of the m_+-columns $\{c_{+,k}\}_1^{m_+}$ and $\mathbb{C}_-^{m_-}$ of the m_--columns $\{c_{-,k}\}_1^{m_-}$. The quadratic form $\frac{1}{i}\Delta_*$ becomes a Hermitian diagonal form, canonical up to the factor 2κ, in the complex linear space $\mathbb{C}^{m_+ + m_-}$ that is a direct sum of $\mathbb{C}_+^{m_+}$ and $\mathbb{C}_-^{m_-}$, $\mathbb{C}^{m_+ + m_-} = \mathbb{C}_+^{m_+} + \mathbb{C}_-^{m_-}$, giving contributions to $\frac{1}{i}\Delta_*$ of the opposite signs. The deficiency indices m_+ and m_- define the signature of this quadratic form $\operatorname{sign}\frac{1}{i}\Delta_* = (m_+, m_-)$, being its inertia indices. In this terms, we can repeat all the arguments of the previous section leading to the main theorem with the same conclusions. We repeat them in the end of the present consideration in new terms.

We now note that we can choose an arbitrary mixed basis $\{e_k\}_1^{m_+ + m_-}$ in the direct sum $D_+ + D_-$ such that

$$\psi_+ + \psi_- = \sum_{k=1}^{m_+ + m_-} c_k e_k$$

which respectively changes the basis in $\mathbb{C}^{m_+ + m_-}$, and the form Δ_* becomes

$$\Delta_*(\psi_*) = 2i\kappa \sum_{k=1}^{m_+ + m_-} \overline{c_k} \omega_{kl} c_l \, , \; \omega_{kl} = \overline{\omega}_{kl} \, , \tag{175}$$

such that $\frac{1}{i}\Delta_*$ becomes the general Hermitian quadratic form, of course, with the same signature. We then diagonalize this form and repeat the above arguments with the known conclusions.

To be true, the second observation includes a suggestion. We know that in the case of differential operators, the asymmetry form Δ_* is determined by the finite boundary values of the local form $[\psi_*, \psi_*]$ that is a form in terms of $\psi_*(x)$ and its derivatives, see (70) and (73),

$$\begin{aligned}
&\Delta_*(\psi_*) = [\psi_*, \psi_*](b) - [\psi_*, \psi_*](a) \, , \\
&[\psi_*, \psi_*](a) = \lim_{x \to a} [\psi_*, \psi_*](x) \, , \; [\psi_*, \psi_*](b) = \lim_{x \to b} [\psi_*, \psi_*](x)
\end{aligned}$$

we repeat (90) and (91). For brevity, we call $[\psi_*, \psi_*](a)$ and $[\psi_*, \psi_*](b)$ the boundary forms. We certainly know that the boundary form at a regular end is a finite nonzero form of order n with respect to finite boundary values of functions and their derivatives of order up to $n-1$ for a differential expression $\check{f}$ of order n. For a singular end, the evaluation of the respective boundary form is generally nontrivial. The suggestion is that the boundary form is expressed in terms of finite number coefficients in front of generally divergent or infinitely oscillating leading asymptotic terms of functions and their derivatives at the end. Therefore, in the general case, boundary forms are expressed in terms of boundary values and the the coefficients describing the asymptotic boundary behavior of functions. For brevity, we call the whole set of the relevant boundary values and the above-introduced coefficients the abv-coefficients (asymptotic boundary value coefficients). Let the p-column $\{c_k\}_1^p$ denote the abv-coefficients for $\psi_* \in D_*$.These columns form a complex linear space $\mathbb{C}^p$, and Δ_* is a finite quadratic anti-Hermitian form in this space

$$\Delta_*(\psi_*) = 2i\kappa \sum_{k=1}^{p} \overline{c}_k \omega_{kl} c_l \, , \; \omega_{kl} = \overline{\omega}_{kl}. \tag{176}$$

It is now sufficient to compare (176) with (175) and repeat the above consideration with the known conclusions on the possibility of s.a. extensions of $\hat{f}^{(0)}$ and their specification in terms of the abv-coefficients by passing to linear combinations $\{c_{+,k}\}_1^{m_+}$ and $\{c_{-,k}\}_1^{m_-}$, $p = m_+ + m_-$, diagonalizing form (176). We call them the diagonal abv-coefficients. All the just said is quite natural. Of course, the nonzero contributions to Δ_* are due to the deficient subspaces, but only the abv-coefficients of functions in $D_+ + D_-$ are relevant, the deficiency indices are evidently identified with the signature of the form $\frac{1}{i}\Delta_*$, and the isometries $\hat{U} : D_+ \to D_-$ reveal themselves as isometries of one set of diagonal boundary values, for example, $\{c_{+,k}\}_1^{m_+}$ to another set $\{c_{-,k}\}_1^{m_-}$. We formulate the conclusions in terms of abv-coefficients in the end of our consideration.

The alternative method is a result of obviously joining the two observations. We outline the consecutive steps of the method for a differential expression $\check{f}$ of order n.

The first step is evaluating the behavior of functions $\psi_*(x) \in D_*$ near the singular ends and either proving that the respective boundary forms vanish identically by establishing the asymptotic behavior of functions at the ends or establishing the asymptotic terms that give nonzero contributions to the respective boundary forms. Unfortunately, there is no universal recipe for performing the both procedures at present. We only give some instructive examples below. As we already said above, the result must be a representation (176) of Δ_* in terms of abv-coefficients $\{c_k\}_1^p$.

The next step consists in diagonalizing the obtained form (176), i.e., diagonalizing the Hermitian matrix ω. As a result, Δ_* becomes a diagonal quadratic form (174) in terms of diagonal abv-coefficients, $\{c_{+,k}\}^{m_+}$ and $\{c_{-,k}\}^{m_-}$, $m_+ + m_- = p$. The resulting conclusions are actually a repetition of the main theorem in the case of finite deficiency indices. Namely, if the inertia indices m_+ and m_- of form (174) are different, $m_+ \neq m_-$, there is no s.a. operators associated with a given s.a. differential expression $\check{f}$. If $m_+ = m_- = 0$, i.e., if $\Delta_* = 0$, the initial symmetric operator $\hat{f}^{(0)}$ is essentially s.a., and there is a unique s.a. operator associated with $\check{f}$ that is given by the closure $\hat{f}$ of $\hat{f}^{(0)}$ coinciding with the adjoint $\hat{f}^* : \hat{f} = \hat{f}^+ = \hat{f}^*$. If $m_+ = m_- = m > 0$, there is an m^2-parameter $U(m)$-family $\left\{\hat{f}_U\right\}$, $U \in U(m)$, of s.a. operators associated with $\check{f}$. Any s.a. $\hat{f}_U$ is specified by s.a. boundary conditions defined by a unitary $m \times m$ matrix U relating the diagonal boundary values $\{c_{+,k}\}_1^m$ and $\{c_{-,k}\}_1^m$ and given by

$$c_{-,k} = U_{kl} c_{+,k}\,,\ k = 1, \ldots, m\,. \tag{177}$$

In the case of singular ends, these boundary conditions have a form of asymptotic boundary conditions prescribing the asymptotic form of functions $\psi_U \in D_{f_U}$ at the singular ends.

A comparative advantage of the method is that it avoids explicitly evaluating the deficient subspaces and deficiency indices, the deficiency indices are obtained by passing. Unfortunately, it is not universal because at present we don't know a universal method for evaluating the asymptotic behavior of functions in D_* at singular ends.

We now consider possible applications of the proposed alternative method.

We first show in detail , maybe superfluous, how simply the problem of s.a. differential expression $\check{p}$ (38) on an interval (a, b) is solved by the alternative method. We recall that the illustration of the conventional methods by the example of $\check{p}$ presented at the end of the previous section was rather extensive. In this case, $[\psi_*, \psi_*] = -i\,|\psi_*|^2$, see (42), therefore, the quadratic asymmetry form Δ_* is $\Delta_*(\psi_*) = -i\,|\psi_*(b)|^2 + i\,|\psi_*(a)|^2$, and $\psi_* \in D_*$ implies $\psi_*, \psi_*' \in L^2(a, b)$.

Let $(a, b) = (-\infty, \infty)$, the whole real axis. The finiteness of the boundary form $[\psi_*, \psi_*](\infty)$ means that $|\psi_*|^2 \to C(\psi_*)$, $x \to \infty$, $|C(\psi_*)| < \infty$, where $C(\psi_*)$ is a finite constant. But this constant must be zero, because $C(\psi_*) \neq 0$ contradicts the square intergability of ψ_*. It is easy to see that for the validity of this conclusion, $\psi_* \to 0$ as $x \to \infty$, it is sufficient that ψ_* be square integrable at infinity together with its derivative ψ_*'; actually, we repeat the well-known assertion that if the both ψ_* and ψ_*' are square integrable at infinity, then ψ_* vanishes at infinity. Similarly, we prove that $\psi_* \to 0$ as $x \to -\infty$ and therefore $[\psi_*, \psi_*](-\infty) = 0$ also for any $\psi_* \in D_*$. We finally have that $\Delta_*(\psi_*) \equiv 0$, in particular, sign $\frac{1}{i}\Delta_* = (0, 0)$. This means that there is a unique s.a. operator $\hat{p}$ associated with $\check{p}$ on the real axis and given by (49), which is in a complete agreement with the known fact established here in passing that the deficiency

indices of the initial symmetric operator $\hat{p}^{(0)}$ are $(0,0)$ and therefore, $\hat{p}^{(0)}$ is essentially s.a. and $\hat{p}=\overline{\hat{p}^{(0)}}=\hat{p}^{*}$.

Let $(a,b)=[0,\infty)$. By the previous arguments, we have $[\psi_{*},\psi_{*}](\infty)=0$, while $[\psi_{*},\psi_{*}](0)=-i|\psi(0)|^{2}\neq 0$ in general. Consequently, the Hermitian quadratic form $\frac{1}{i}\Delta_{*}(\psi_{*})=|\psi_{*}(0)|^{2}$ is positive definite and sign $\frac{1}{i}\Delta_{*}=(1,0)$. This means that there is no s.a. operators associated with $\check{p}$ on a semiaxis, which is in complete agreement with the known fact that the deficiency indices of $\hat{p}^{(0)}$ in this case are $(1,0)$.

Let $(a,b)=[0,l]$, a finite segment. In this case, we have $\frac{1}{i}\Delta_{*}=|\psi_{*}(0)|^{2}-|\psi_{*}(l)|^{2}$, a nontrivial Hermitian quadratic form with sign $\frac{1}{i}\Delta_{*}=(1,1)$, which confirms the known fact that the deficiency indices of $\hat{p}^{(0)}$ in this case are $(1,1)$. The corresponding s.a. boundary conditions are

$$\psi(l)=e^{i\vartheta}\psi(0)\ ,\ 0\leq\vartheta\leq 2\pi\,,$$

they define the one-parameter $U(1)$-family $\{\hat{p}_{\vartheta}\}$ of s.a. operators associated with $\check{p}$ on a segment $[0,l]$, the family given by (54).

The case of an even s.a. differential expression with the both regular ends is completely fall into the framework of the alternative method. Let $\check{f}$ be an even s.a. differential expression of order n on a finite interval (a,b), the both ends being regular. In this case, we have representation (157) for the sesquilinear asymmetry form ω_{*}, while the quadratic asymmetry form Δ_{*} is represented as

$$\Delta_{*}(\psi_{*})=\Psi_{*}^{+}(b)\,\mathcal{E}\Psi_{*}(b)-\Psi_{*}^{+}(a)\,\mathcal{E}\Psi_{*}(a)\ , \tag{178}$$

where the matrix $\mathcal{E}$ is given by (124) and $\Psi_{*}(b)$, $\Psi_{*}(b)$ are the columns whose components are the respective boundary values of functions $\psi_{*}\in D_{*}$ and their (quasi)derivatives of order up to $n-1$,

$$\Psi_{*}(a)=\begin{pmatrix}\psi_{*}(a)\\ \psi_{*}^{[1]}(a)\\ \vdots\\ \psi_{*}^{[n-1]}(a)\end{pmatrix},\ \Psi_{*}(b)=\begin{pmatrix}\psi_{*}(b)\\ \psi_{*}^{[1]}(b)\\ \vdots\\ \psi_{*}^{[n-1]}(b)\end{pmatrix}, \tag{179}$$

or $\Psi_{*k}(a)=\psi_{*}^{[k-1]}(a)$, $\Psi_{*k}(b)=\psi_{*}^{[k-1]}(b)$, $k=1,...,n$, an analogue of (126).

An important preliminary remark concerning dimensional considerations is in order here. In the mathematical literature, the variable x is considered dimensionless, such that $\psi_{*},\psi_{*}^{[1]},...,\psi_{*}^{[n-1]}$ have the same zero dimension as well as the differential expression $\check{f}$ itself. Therefore, comparing (178) with (176), where $p=2n$ and $\kappa=1$, as it is conventionally adopted in the mathematical literature, we could immediately identify the set $\{c_{k}\}_{1}^{2n}$ with the set $\left\{\psi_{*}^{[k-1]}(a)\right\}_{1}^{n}\cup\left\{\psi_{*}^{[k-1]}(b)\right\}_{1}^{n}$, the matrix ω is then given by

$$\omega=\frac{1}{2i}\begin{pmatrix}-\mathcal{E} & 0\\ 0 & \mathcal{E}\end{pmatrix}. \tag{180}$$

But in physics, the variable x is usually assigned a certain dimension, the dimension of length, which we write as $[x]=[\text{length}]$, while functions ψ_{*} have dimension of the square root of inverse length, $[\psi_{*}]=[\text{length}]^{-1/2}$. Therefore, $\psi_{*}^{[k]}(x)$ has the dimension $\left[\psi_{*}^{[k]}\right]=[\text{length}]^{-k-1/2}$, and if the coefficient function $f_{n}(x)$ in $\check{f}$ is taken dimensionless, the $\check{f}$ itself is assigned the dimension $\left[\check{f}\right]=[\text{length}]^{-n}$. It is convenient to have all variables c_{k}, $k=1,\ldots,2n$, in (176) of

equal dimension in order the matrix elements of the unitary matrix U in (177) be dimensionless. This can be done as follows.

We introduce arbitrary, but fixed, parameter τ of dimension of length, $[\tau] = [\text{length}]$, and represent $\Delta_*(\psi_*)$ as[58]

$$\Delta_*(\psi_*) = \tau^{-n+1}\left[\Psi_\tau^+(b)\,\mathcal{E}\Psi_\tau(b) - \Psi_\tau^+(a)\,\mathcal{E}\Psi_\tau(a)\right], \tag{181}$$

where

$$\Psi_\tau(a) = \begin{pmatrix} \psi_*(a) \\ \tau\psi_*^{[1]}(a) \\ \vdots \\ \tau^{n-1}\psi_*^{[n-1]}(a) \end{pmatrix}, \ \Psi_\tau(b) = \begin{pmatrix} \psi_*(b) \\ \tau\psi_*^{[1]}(b) \\ \vdots \\ \tau^{n-1}\psi_*^{[n-1]}(b) \end{pmatrix}$$

or in components

$$\Psi_{\tau k}(a) = \tau^{k-1}\psi_*^{[k-1]}(a)\ ,\ \Psi_{\tau k}(b) = \tau^{k-1}\psi_*^{[k-1]}(b)\ ,\ k = 1,\dots,n\,,$$

the dimension of $\Psi_\tau(a)$ and $\Psi_\tau(b)$ is $[\Psi_\tau] = [\text{length}]^{-1/2}$.

We can now identify the set $\{c_k\}_1^{2n}$ with $\Psi_\tau(a) \cup \Psi_\tau(b)$ and proceed to diagonalizing quadratic form (181) or matrix ω (180). Diagonalizing is evidently reduced to separately diagonalizing the quadratic form $\Psi_\tau^+(a)\,\mathcal{E}\Psi_\tau(a)$ and $\Psi_\tau^+(b)\,\mathcal{E}\Psi_\tau(b)$ or to diagonalizing the matrix $\mathcal{E}$. But this was already done above, see formulas (154), (155), and (156). The final result is

$$\Delta_*(\psi_*) = 2i\kappa\left[\Psi_{\tau(+-)}^+\Psi_{\tau(+-)} - \Psi_{\tau(-+)}^+\Psi_{\tau(-+)}\right], \tag{182}$$

where $\kappa = 1/4\tau^{-n+1}$ and $\Psi_{\tau(+-)}$, $\Psi_{\tau(-+)}$ are the n-columns

$$\Psi_{\tau(+-)} = \begin{pmatrix} \Psi_{\tau+}(b) \\ \Psi_{\tau-}(a) \end{pmatrix},\ \Psi_{\tau(-+)} = \begin{pmatrix} \Psi_{\tau-}(b) \\ \Psi_{\tau+}(a) \end{pmatrix},$$

where $\Psi_{\tau\pm}(a)$, are the $n/2$-columns

$$\Psi_{\tau+}(a) = \begin{pmatrix} \psi_*(a) + i\tau^{n-1}\psi_*^{[n-1]}(a) \\ \tau\psi_*^{[1]}(a) + i\tau^{[n-2]}\psi_*^{[n-2]}(a) \\ \vdots \\ \tau^{n/2-1}\psi_*^{[n/2-1]}(a) + i\tau^{n/2}\psi_*^{[n/2]}(a) \end{pmatrix}, \tag{183}$$

$$\Psi_{\tau-}(a) = \begin{pmatrix} \tau^{n/2-1}\psi_*^{[n/2-1]}(a) - i\tau^{n/2}\psi_*^{[n/2]}(a) \\ \vdots \\ \tau\psi_*^{[1]}(a) - i\tau^{n-2}\psi_*^{[n-2]}(a) \\ \psi_*(a) - i\tau^{n-1}\psi_*^{[n-1]}(a) \end{pmatrix}, \tag{184}$$

or in components

$$\Psi_{\tau+,k}(a) = \tau^{k-1}\psi_*^{[k-1]}(a) + i\tau^{n-k}\psi_*^{[n-k]}(a)\ ,\ k = 1,\dots,n/2\,, \tag{185}$$

$$\Psi_{\tau-,k}(a) = \tau^{n/2-k}\psi_*^{[n/2-k]}(a) - i\tau^{n/2+k-1}\psi_*^{[n/2+k-1]}(a)\ ,\ k = 1,\dots,n/2\,. \tag{186}$$

[58]The dimension of Δ_* is $[\Delta_*] = [\text{length}]^{-n}$.

We note that $\Psi_{\tau-,k}(a)$ are obtained from $\Psi_{\tau+,k}(a)$ by the change $i \to -i$, and $k \to n/2+1-k$. The $n/2$-columns $\Psi_{\tau\pm,k}(b)$ are given by similar formulas with the change $a \to b$. In other words, the components of the n-columns $\Psi_{\tau(+-)}$ and $\Psi_{\tau(-+)}$ are respectively given by

$$\Psi_{\tau(+-)k} = \begin{cases} \tau^{k-1}\psi_*^{[k-1]}(b) + i\tau^{n-k}\psi_*^{[n-k]}(b)\,, \ k = 1, \ldots, n/2\,, \\ \tau^{n-k}\psi_*^{[n-k]}(a) - i\tau^{k-1}\psi_*^{[k-1]}(a)\,, \ , \ k = n/2+1, \ldots, n\,, \end{cases}$$

and

$$\Psi_{\tau(-+)k} = \begin{cases} \tau^{n/2-k}\psi_*^{[n/2-k]}(b) - i\tau^{n/2+k-1}\psi_*^{[n/2+k-1]}(b)\,, \ k = 1, \ldots, n/2\,, \\ \tau^{k-n/2-1}\psi_*^{[k-n/2-1]}(a) + i\tau^{3n/2-k}\psi_*^{[3n/2-k]}(a)\,, \ , \ k = n/2+1, \ldots, n\,. \end{cases}$$

It follows from (182) that the s.a. boundary conditions defining a s.a. operator $\hat{f}_U$ associated with $\check{f}$ are given by

$$\Psi_{\tau(-+)} = U\Psi_{\tau(+-)}\,, \tag{187}$$

where U is an $n \times n$ unitary matrix, $U \in U(n)$. When U ranges over all $U(n)$ group, we cover the whole n^2-parameter $U(n)$-family $\left\{\hat{f}_U\right\}$ of s.a. operators associated with a given s.a. deferential expression $\check{f}$ or order n on a finite interval (a, b) with the both regular ends.

We conclude this item with some evident remarks.

1) We use the same symbol $\hat{f}_U$ for the notation of s.a. extensions as before, although the subscript U has now another meaning. In the previous context, the subscript U was a symbol of a an isometry $\hat{U} : D_+ \to D_-$, in the present context, it is a symbol of a unitary mapping (187) of one set of boundary values to another one.

2) We could organize the column $\Psi_{\tau(-+)}$ in another way, for example,

$$\Psi_{\tau(-+)} = \begin{pmatrix} \Psi_{\tau-}(b) \\ \Psi_{\tau+}(a) \end{pmatrix} \to \Xi\Psi_{\tau(-+)} = \begin{pmatrix} \Psi_{\tau+}(a) \\ \Psi_{\tau-}(b) \end{pmatrix},$$

where the unitary matrix Ξ is $\Xi = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$, here, I is the $n/2 \times n/2$ unit matrix, $\Xi^2 = I$. Then U in (187) would change to ΞU, which is also a unitary matrix.

3) It is evident that we can specify s.a. boundary conditions by $\Psi_{\tau(+-)} = U\Psi_{\tau(-+)}$. It is sufficient to make the change $U \to U^{-1}$ in (187).

4) If a matrix U in (187) is of a specific block-diagonal form

$$U = \begin{pmatrix} U(b) & 0 \\ 0 & U^{-1}(a) \end{pmatrix}, \tag{188}$$

where $U(a)$ and $U(b)$ are $n/2 \times n/2$ unitary matrices[59], we obtain the so-called splitted s.a. boundary conditions

$$\Psi_{\tau-}(a) = U(a)\Psi_{\tau+}(a)\,, \ \Psi_{\tau-}(b) = U(b)\Psi_{\tau+}(b)\,, \tag{189}$$

For illustration, we consider the familiar second-order differential expression $\check{H}$ (65) on a segment $[0, l]$ with an integrable potential V which implies that the both ends are regular. This

[59]For convenience, we take the down right block in r.h.s. of (188) in the form $U^{-1}(a)$ rather than $U(a)$; see below (189).

includes the case of a free particle where $V=0$ and $\check{H}=\check{H}_0$ (94). The s.a. boundary conditions in this case are given by

$$\begin{pmatrix} \psi(l)-i\tau\psi'(l) \\ \psi(0)+i\tau\psi'(0) \end{pmatrix} = U \begin{pmatrix} \psi(l)+i\tau\psi'(l) \\ \psi(0)-i\tau\psi'(0) \end{pmatrix},$$

where U is an 2×2 unitary matrix, to our knowledge, they were first given in [33] with $\tau=l$.

Choosing $U=I$, we obtain s.a. boundary conditions (132): $\psi'(0)=\psi'(l)=0$.

With $U=-I$, we reproduce s.a. boundary conditions (131): $\psi(0)=\psi(l)=0$.

If

$$U=\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\vartheta} \end{pmatrix},\ -\pi\leq\theta,\ \vartheta\leq\pi,$$

we obtain splitted s.a. boundary condition (160): $\psi'(0)=\lambda\psi(0)$, $\psi'(l)=\lambda\psi(l)$, where $\lambda=-\frac{1}{\tau}\tan\frac{\vartheta}{2}$, $\mu=-\frac{1}{\tau}\tan\frac{\theta}{2}$, $-\infty\leq\lambda,\ \mu\leq\infty,\ -\infty\backsim\infty$.

Choosing

$$U=\begin{pmatrix} 0 & e^{i\vartheta} \\ e^{-i\vartheta} & 0 \end{pmatrix},$$

we obtain modified periodic s.a. boundary conditions (161): $\psi(l)=e^{i\vartheta}\psi(0)$, $\psi'(l)=e^{i\vartheta}\psi'(0)$.

Finally, taking $\tau=l/\pi$ and

$$U=-\frac{1}{\cosh\pi}\begin{pmatrix} i\sinh\pi & 1 \\ 1 & i\sinh\pi \end{pmatrix},$$

we reproduce "exotic" s.a. boundary conditions (130).

Another case where the alternative method is efficient is the case of an even differential expression $\check{f}$ of order n with one regular end, let it be a, and one singular end, b, if the boundary forms vanish identically at the singular end, in particular, $[\psi_*,\psi_*](b)\equiv 0$. In this case, the quadratic asymmetry form Δ_* is, see (182) with $\Psi_{\tau\pm}(b)=0$,

$$\Delta_*(\psi_*)=2i\kappa\left[\Psi_{\tau-}^{+}(a)\,\Psi_{\tau-}(a)-\Psi_{\tau+}^{+}(a)\,\Psi_{\tau+}(a)\right], \tag{190}$$

where the $n/2$-columns of boundary values are given by (183)–(186). It follows from (190) that s.a. boundary conditions defining a s.a. operator $\hat{f}_U$ associated with $\check{f}$ are given by[60]

$$\Psi_{\tau-}(a)=U\Psi_{\tau+}(a), \tag{191}$$

where U is an unitary matrix, $U\in U(n/2)$. When U ranges over all group $U(n/2)$, we cover the whole $(n/2)^2$-parameter $U(n/2)$-family $\left\{\hat{f}_U\right\}$ of associated s.a. operators in the case under consideration.

We know from the above considerations, see Lemma 13 that the sufficient condition for vanishing the boundary forms at the singular end is that the deficiency indices of the initial associated symmetric operator $\hat{f}^{(0)}$ be minimum, $(n/2,n/2)$. But formula (190) explicitly shows

[60] Of course, we can interchange $\Psi_{\tau_-}(a)$ and $\Psi_{\tau+}(a)$ in (191). We can also repeat the remark after formula (187) concerning the new meaning of the symbol $\hat{f}_U$.

that conversely, if the boundary form $[\psi_*, \psi_*](b)$ vanishes identically, the signature of the Hermitian form $\frac{1}{i}\Delta_*$ is

$$\operatorname{sign}\frac{1}{i}\Delta_* = (n/2, n/2)\ . \tag{192}$$

which means that the deficiencies indices of $\hat{f}^{(0)}$ are $(n/2, n/2)$. In other words, we can state that for an even s.a. differential expression $\check{f}$ of order n with one regular and one singular end, the deficiency indices of the associated initial symmetric operator $\hat{f}^{(0)}$ are $(n/2, n/2)$ iff the boundary forms at the singular end identically vanish. Therefore, for such differential expressions, the description of the associated s.a. differential operators by s.a. boundary conditions (191) is in complete agreement with the previous description given by Theorem 14 and Theorem 18. We only note that the application of Theorem 14 requires evaluating the deficient subspaces and that the matrix $A_{1/2}$ in Theorems 18 is defined up to the change $A_{1/2} \to A_{1/2}Z$, where Z is a nonsingular matrix, while s.a. boundary conditions (191) avoid evaluating the deficient subspaces and contain no arbitrariness.

For illustration, we consider the same differential expression $\check{H}$ (65) on the semiaxis $[0, \infty)$ with a potential V integrable at the origin, such that the left end is regular. We know the two criteria given by respective (167) and (168) for the initial symmetric operator $\hat{H}^{(0)}$ to have the deficiency indices $(1, 1)$ and, therefore, the boundary form $[\psi_*, \psi_*](\infty)$ to vanish identically. In the spirit of the alternative method, we now directly, without addressing to deficiency indices, show that under either of conditions (167) or (168), we have $[\psi_*, \psi_*](\infty) \equiv 0$.

We begin with condition[61] (167). The corresponding assertion is based on the observation that under this condition, the function $x^{-1/2}\psi_*'$ is bounded for $x > a > 0$,

$$\left|x^{-1/2}\psi_*'\right| < C'(\psi_*) < \infty\,,\ x > a > 0,\ \forall\psi_* \in D_*\,. \tag{193}$$

It follows that the function $x^{-1/2}\overline{\psi_*}\psi_*'$ is square integrable at infinity as well as ψ_*, therefore, the function $x^{-1/2}[\psi_*, \psi_*] = x^{-1/2}\left(\overline{\psi_*'}\psi_* - \overline{\psi_*}\psi_*'\right)$ is also square integrable at infinity. On the other hand, the finiteness of the boundary form $[\psi_*, \psi_*](\infty)$,

$$[\psi_*, \psi_*] \to C(\psi_*)\,,\ x \to \infty\,,\ |C(\psi_*)| < \infty\,, \tag{194}$$

implies $x^{-1/2}[\psi_*, \psi_*] \to x^{-1/2}C(\psi_*)\ ,\ x \to \infty$. But the function in l.h.s. is square integrable at infinity, whereas the function in r.h.s. is not unless $C(\psi_*) = 0$, which proves that $[\psi_*, \psi_*](\infty) \equiv 0$. It remains to prove (193).

For this, we recall that $\psi_* \in D_*$ implies $\psi_*, -\psi_*'' + V\psi_* \in L^2(0, \infty)$ which in turn implies that the function $\int_a^x d\xi\, |\chi_*|^2$, where $\chi_* = -\psi_*'' + V\psi_*$, is bounded, $\int_a^x d\xi\, |\chi_*|^2 < C_1(\chi_*) < \infty\,,$ therefore,

$$\left|\int_a^x d\xi\chi_*\right| < C_1^{1/2}(\chi_*)\sqrt{x-a}\,,\ x > a\,, \tag{195}$$

by the Cauchy–Bounjakowsky inequality. If $V \in L^2(0, \infty)$ as well as ψ_*, the function $V\psi_*$ is integrable on $[0, \infty)$, and therefore, the function $\int_a^x d\xi V\psi_*$ is bounded on $[0, \infty)$,

$$\left|\int_a^x d\xi V\psi_*\right| < C_2(\chi_*) < \infty\,. \tag{196}$$

[61] We have already mentioned that this condition implies the integrability of $V(x)$ at the origin.

Integrating the equality $-\psi_*'' + V\psi_* = \chi_*$, we have

$$\psi_*'(x) = \int_a^x d\xi V\psi_* - \int_a^x d\xi \chi_* + \psi_*'(a) \ ,$$

and then using (195) and (196), we obtain the inequality

$$|\psi_*'| < C_2(\psi_*) + C_1^{1/2}(\psi_*)\sqrt{x-a} + |\psi_*'(a)| \ , \ x > a \, , \ \forall\psi_* \in D_* \, ,$$

which yields (193) and proves the assertion.

The important concluding remark is that as the given proof shows, in order that the boundary form $[\psi_*, \psi_*](\infty)$ vanish identically, condition (167) can be weakened: it is sufficient that the potential V be square integrable at infinity, i.e., $V \in L^2(a, \infty)$ with some $a > 0$.

We now turn to condition (168). The corresponding assertion is based on the observation that under this condition, the function ψ_*'/x is square integrable at infinity as well as ψ_*,

$$\int_a^\infty d\xi \left|\frac{\psi_*'}{\xi}\right|^2 < \widetilde{C}'(\psi_*) < \infty \, , \ a > 0 \, , \ \forall\psi_* \in D_* \, . \tag{197}$$

It follows that the function $\overline{\psi_*}\psi_*'/x$ is integrable at infinity, and, therefore, the function $x^{-1}[\psi_*, \psi_*] = x^{-1}\left(\overline{\psi_*'}\psi_* - \overline{\psi_*}\psi_*'\right)$ is also integrable at infinity. On the other hand, the finiteness of the boundary form $[\psi_*, \psi_*](\infty)$, see (194), implies that $x^{-1}[\psi_*, \psi_*] \to C(\psi_*)x^{-1}$ as $x \to \infty$. But the function in l.h.s. is integrable at infinity, whereas the function in r.h.s. is not unless $C(\psi_*) = 0$, which proves that $[\psi_*, \psi_*](\infty) = 0$. It remains to prove (197).

The proof is by contradiction. We first make some preliminary estimates, as in the proof of the previous assertion, based on the conditions $\psi_*, -\psi_*'' + V\psi_* = \chi_* \in L^2(0,a)$. These conditions imply that $\int_a^x d\xi |\psi_*|^2 < C_1(\psi_*) < \infty$, we already used this estimate before, and that

$$\begin{aligned}
&\int_a^x d\xi \frac{|\psi_*|^2}{\xi^3} < C_3(\psi_*) < \infty \, , \ \int_a^x d\xi \frac{|\psi_*|^2}{\xi^4} < C_4(\psi_*) < \infty \, , \ a > 0 \, , \\
&\left|\int_a^x d\xi \left(\overline{\chi_*}\frac{\psi_*}{\xi^2}\psi_* + \frac{\overline{\psi_*}}{\xi^2}\chi_*\right)\right| < 2C_1^{1/2}(\chi_*)C_4^{1/2}(\psi_*) \, .
\end{aligned} \tag{198}$$

The condition (168) means that there exist some $a > 0$ such that $V(x)/x^2 > -K$, $K > 0$, and, therefore,

$$\int_a^x d\xi \frac{V}{\xi^2}|\psi_*|^2 > -K\int_a^x d\xi |\psi_*|^2 > -KC_1(\psi_*) \ . \tag{199}$$

On the other hand, we have

$$\overline{\psi_*}\chi_* + \psi_*\overline{\chi_*} = -\frac{d^2}{dx^2}|\psi_*|^2 + 2|\psi_*'|^2 + 2V|\psi_*|^2 \ .$$

Multiplying this equality by $1/x^2$ and integrating with integrating the term $-x^{-2}d^2/dx^2|\psi_*|^2$ by parts, we obtain that

$$\begin{aligned}
&\frac{1}{x^2}\frac{d}{dx}|\psi_*|^2 = 2\int_a^x d\xi \left|\frac{\psi_*'}{\xi}\right|^2 + 2\int_a^x d\xi \frac{V}{\xi^2}|\psi_*|^2 - 6\int_a^x d\xi \frac{|\psi_*|^2}{\xi^4} - \int_a^x d\xi \left(\overline{\chi_*}\psi_* + \overline{\psi_*}\chi_*\right) \\
&-2\frac{|\psi_*|^2}{x^3} + C_5(\psi_*) \ , \ C_5(\psi_*) = \left.\left(\frac{1}{x^2}\frac{d}{dx}|\psi_*|^2 + \frac{2}{x^3}|\psi_*|^2\right)\right|_{x=a} \, .
\end{aligned}$$

In view of (198) and (199), this yields the inequality

$$\frac{d}{dx}\left|\psi_{*}\right|^{2}>x^{2}\left(2\int_{a}^{x}d\xi\left|\frac{\psi_{*}^{\prime}}{\xi}\right|^{2}-C_{6}\left(\psi_{*}\right)\right)-2\frac{\left|\psi_{*}\right|^{2}}{x^{3}}\,,$$

where $C_6 = 2KC_1(\psi_*) + 6C_4(\psi_*) + 2C_1^{1/2}(\chi_*)\, C_4^{1/2}(\psi_*) - C_5(\psi_*)$. Let now the integral $I(x) = \int_a^x d\xi \left|\frac{\psi_*'}{\xi}\right|^2$ diverge as $x \to \infty$. Then for sufficiently large x, $x > b > a$, we have $2I(x) - C_6(\psi_*) > C_7(\psi_*) > 0$, and, therefore, we obtain the inequality

$$\frac{d}{dx}\left|\psi_{*}\right|^{2}>x^{2}C_{7}\left(\psi_{*}\right)-2\frac{\left|\psi_{*}\right|^{2}}{x^{3}}\,.$$

Again, integrating this inequality and taking (198) into account, we find $\left|\psi_*\right|^2 > C_7(\psi_*)\, x^3/3 - C_8(\psi_*)$, where $C_8(\psi_*) = 2C_3(\psi_*) + C_7(\psi_*)\, b^3/3 - \left|\psi_*\right|^2(b)$, whence it follows that $\left|\psi_*\right|^2 \to \infty$ as $x \to \infty$, which contradicts the square integrability of ψ_* at infinity. This contradiction proves that the function ψ_*'/x is square integrable at infinity, i.e., (197) holds, and thus proves the assertion. We should not forget that because the sesquilinear and quadratic forms define each other, the vanishing of the boundary form $[\psi_*, \psi_*]$ implies the vanishing of the sesquilinear boundary form $[\chi_*, \psi_*]$, and vice versa.

The proved criteria for vanishing the boundary forms at infinity allows formulating the assertion that the s.a. operators associated with s.a. differential expression $\check{H}$ (65) on the semiaxis $[0, \infty)$ with a potential V integrable at the origin and satisfying either the condition that it is also square integrable at infinity or the condition that $V(x) > -Kx^2$, $K > 0$, for sufficiently large x are specified by s.a. boundary conditions given by

$$\psi\left(0\right)-i\tau\psi^{\prime}\left(0\right)=e^{i\vartheta}\left[\psi\left(0\right)+i\tau\psi^{\prime}\left(0\right)\right]\,,\ -\pi\leq\vartheta\leq\pi\,, \tag{200}$$

which is equivalent to

$$\psi^{\prime}\left(0\right)=\lambda\psi\left(0\right)\,,\ \lambda=-\frac{1}{\tau}\tan\frac{\vartheta}{2},\ -\infty\leq\lambda\leq\infty\,,$$

the both $\lambda = \pm\infty$ yield the same s.a. boundary condition $\psi(0) = 0$: the whole family $\left\{\hat{H}_\lambda\right\}$ of s.a. operators associated with $\check{H}$ is not the real axis, but a circle. We thus reproduce the previous result given by (169).

The above criteria are evidently extended to the case of the same differential expression $\check{H}$ (65), but now on the whole real axis $\mathbb{R}^1 = (-\infty, \infty)$, providing the vanishing of the boundary forms on the both infinities. This allows immediately formulating a similar assertion for this case: if a potential $V(x)$ is locally integrable and satisfies the two alternative conditions that V is either square integrable at minus infinity or $V(x) > -K_- x^2$, $K_- > 0$, for sufficiently large negative x and V is either square integrable at plus infinity or $V(x) > -K_+ x^2$, $K_+ > 0$, for sufficiently large x (generally K_- and K_+ may be different), then there is a unique s.a. operator $\hat{H}$ associated with $\check{H}$, it is given by the closure of the initial symmetric operator $\hat{H}^{(0)}$ defined on the natural domain, $\hat{H} = \overline{\hat{H}^{(0)}} = \hat{H}^*$.

The case of a free particle where $V = 0$ and $\check{H} = \check{H}_0$ certainly falls under the above conditions, such that $\hat{H}_0$ defined on natural domain (95) is really s.a. as we said in advance in

subsec. 3.4. It may be also useful to mention that in this case we can strengthen the estimates on the asymptotic behavior of functions $\psi_*(x) \in D_{0*}$, namely, $\psi_*(x), \psi_*'(x) \to 0$ as $|x| \to \infty$. For this, it is sufficient to prove that ψ_*' is square integrable both at plus and minus infinity, which means that $\psi_*' \in L^2(-\infty, \infty)$ as well as ψ_* and ψ_*''. It then remains to refer to the assertion that we obtained when considering the case of the differential expression $\check{p}$ (38): if ψ_*, ψ_*' are square integrable at infinity, plus or minus, this implies that ψ_* vanishes at infinity, and to apply this assertion to the respective pairs ψ_*, ψ_*' and ψ_*', ψ_*''. We only prove that if $\psi_* \in D_{0*}$, ψ_*' is square integrable at $+\infty$; the proof for $-\infty$ is completely similar. The proof is by contradiction. The condition $\psi_* \in D_{0*}$ implies that ψ_* and ψ_*'' are square integrable at infinity; therefore, the integral $\int_a^x d\xi \left(\overline{\psi_*}\psi_*'' + \overline{\psi_*''}\psi_*\right)$ is convergent as $x \to \infty$,

$$\int_a^x d\xi \left(\overline{\psi_*}\psi_*'' + \overline{\psi_*''}\psi_*\right) \to C(\psi_*) \ , \ x \to \infty \, , \ |C(\psi_*)| < \infty \, .$$

On the other hand

$$\int_a^x d\xi \left(\overline{\psi_*}\psi_*'' + \overline{\psi_*''}\psi_*\right) = \frac{d}{dx}|\psi_*|^2 - 2\int_a^x d\xi \, |\psi_*'|^2 - \left.\frac{d}{dx}|\psi_*|^2\right|_{x=a} .$$

and if $\int_a^x d\xi \, |\psi_*'|^2 \to \infty$ as $x \to \infty$, then $\frac{d}{dx}|\psi_*|^2 \to \infty$ as $x \to \infty$ also, and therefore, $|\psi_*|^2 \to \infty$ as $x \to \infty$, which contradicts the square intergability of ψ_* and proves the required.

We have thus completely paid our debt since subsec. 3.4.

We again note that in the above consideration related to $\check{H}$ on the whole axis, we escape evaluating the deficient subspaces and deficient indices, but, in passing, we obtain that the deficiency indices of $\hat{H}^{(0)}$ are $(0,0)$, and therefore, $\hat{H}^{(0)}$ is essentially s.a..

It remains to demonstrate how the alternative method can work in the case of singular ends. For illustration, we take the differential expression $\check{H} = -d^2/dx^2 - \alpha/x^2$ on the positive semiaxis $[0, \infty)$ with the dimensionless coupling constant $\alpha > 1/4$. This differential expression can be identified with the radial Hamiltonian $\check{H}_l$ (96), (97) for a three-dimensional particle in the field of a strongly attractive central potential $V = -\frac{\alpha}{r^2}$ with $l = 0$ (the s-wave) or $V = -\frac{\alpha + l(l+1)}{r^2}$ with $l \neq 0$ (the higher waves); such a potential yields a phenomenon known as the "fall to a center". Historically, this was the first case where the standard textbook approach did not allow constructing scattering states and even raised the question on the applicability of quantum mechanics to strongly singular potentials [10].

The potential $V = -\frac{\alpha}{x^2}$ satisfies the both criteria for vanishing the boundary form $[\psi_*, \psi_*](\infty)$, and the problem of constructing s.a. operators associated with $\check{H}$ reduces to the problem of evaluating the boundary form $[\psi_*, \psi_*](0)$. It is solved by the following arguments that can be extended to another cases, and maybe, to the general case, the idea was already stated above, in the consideration related to formula (93). By the definition of the domain D_*, the functions ψ_* and $\chi_* = -\psi_*'' - \alpha/x^2\psi_*$ belong to $L^2(0, \infty)$. This means that $\psi_* \in D_*$ can be considered as a square-integrable solution of the inhomogenous differential equation

$$-\psi_*'' - \alpha/x^2\psi_* = \chi_* \tag{201}$$

with a square-integrable, and therefore, locally integrable, inhomogenous term χ_*. Therefore, as any solution of (201), the function ψ_* can be represented as

$$\psi_* = c_+u_+ + c_-u_- - \frac{1}{2i\mu_0\varkappa}\left[u_+\int_0^x d\xi u_-(\xi)\chi_*(\xi) - u_-\int_0^x d\xi u_+(\xi)\chi_*(\xi)\right] \tag{202}$$

in terms of the two linearly independent solutions $u_{\pm} = (\mu_0 x)^{1/2 \pm i\varkappa}$ of the homogenous equation $-u''_{\pm} - \alpha/x^2 u_{\pm} = 0$, where $\varkappa = \sqrt{\alpha - 1/4} > 0$ and μ_0 is an arbitrary, but fixed, dimensional parameter of dimension of inverse length introduced by dimensional considerations, the factor -$1/2i\mu_0\varkappa$ is the inverse Wronskian of the solutions u_+ and u_-, and $c_{\pm}$ are some constants.

Representation (202) allows easily estimating the asymptotic behavior of ψ_* as $x \to 0$. Using the Cauchy–Bounjakowsky inequality in estimating the integral term in (202), we obtain that the asymptotic behavior of ψ'_* and ψ_* near the origin is given by

$$\begin{aligned} \psi_* &= c_+ u_+ + c_- u_- + (\mu_0 x)^{3/2} \varepsilon(x) , \\ \psi'_* &= \left(\frac{1}{2} + i\varkappa\right) \mu_0 c_+ u_+^{-1} + \left(\frac{1}{2} - i\varkappa\right) \mu_0 c_- u_-^{-1} + (\mu_0 x)^{1/2} \widetilde{\varepsilon}(x) , \end{aligned} \tag{203}$$

where $\varepsilon(x)$, $\widetilde{\varepsilon}(x) \backsim \int_0^x d\xi \, |\chi_*|^2 \to 0$ as $x \to 0$. We note that it is the equally vanishing of the solutions $u_{\pm}$ of the homogenous equation at the origin that caused difficulties in the choice of an acceptable scattering state. Formulas (203) yield $[\psi_*, \psi_*](0) = 2i\mu_0\varkappa \left(|c_+|^2 - |c_-|^2\right)$, whence it immediately follows the s.a. boundary conditions $c_- = c_+ e^{i\vartheta}$, $0 \leq \vartheta \leq 2\pi$, or in the unfolded form,

$$\psi = c(\mu_0 x)^{1/2} \left[(\mu_0 x)^{i\varkappa} + e^{i\vartheta} (\mu_0 x)^{-i\varkappa}\right] + (\mu_0 x)^{3/2} \varepsilon(x) , \tag{204}$$

which have the form of asymptotic boundary conditions.

This asymptotic s.a. boundary conditions can be rewritten as

$$\psi = c(\mu_0 x)^{1/2} \cos[\varkappa \ln(\mu_0 x) - \vartheta/2] + (\mu_0 x)^{3/2} \varepsilon(x) , \tag{205}$$

then the extension parameter ϑ can be treated as the phase of the scattering wave at the origin, or as

$$\psi = c(\mu_0 x)^{1/2} \left[(\mu x)^{i\varkappa} + (\mu x)^{-i\varkappa}\right] + (\mu_0 x)^{3/2} \varepsilon(x) , \tag{206}$$

where the dimensional parameter $\mu = \mu_0 e^{-\vartheta/2\varkappa}$, $\mu_0 e^{-\pi/\varkappa} \leq \mu \leq \mu_0$, plays the role of the extension parameter and manifests a "dimensional transmutation" and also, as can be shown, the breaking of a "naive" scale symmetry of the system: $x \to x/l \Longrightarrow \hat{H} \to l^2 \hat{H}$. We also note that by passing, we obtain that the deficiency indices of $\hat{H}^{(0)}$ are $(1, 1)$.

The conclusion is that in the case under consideration, we have a one-parameter $U(1)$-family $\left\{\hat{H}_\vartheta\right\} = \left\{\hat{H}_\mu\right\}$ of s.a. Hamiltonians associated with $\check{H}$, these are parameterized either by the angle ϑ or the dimensional parameter μ and are specified by asymptotic boundary conditions (204), or (205), or (206). The parameters ϑ or μ enter the theory as additional parameters specifying the corresponding different quantum mechanical systems.

One of the physical consequences of this conclusion for three-dimensional system is that we should realize that if we describe interaction in terms of strongly attractive central potentials, a complete description requires additional specification in terms of new parameters that mathematically reveal itself as extension parameters.

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